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Solid Oxide Fuel Cell design and Application of Formal Methods

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Dedicated to my dad Tesfazghi Hagos
and my mum Rahel Meressi.

ABSTRACT

The design of solid oxide fuel cells has inherent conflicts and compromises due to the mechanical and electrochemical requirements. The design objective is to reduce the fabrication cost of cell components while maintaining high efficiency and reliability. Solid oxide fuel cells have yet to go through a lot of research and development stage before they can be commercialised to replace conventional power generating devices. The cost associated with manufacturing of cells and stack has proved to be prohibitively high at this stage of the development.

To overcome this, a cost effective manufacturing process and associated design was needed. Taguchi method of experimentation was employed to this end. Design Function Deployment (DFD) methodology was used to compare and develop previous conceptual designs and a new combined design is proposed. Mathematical models were developed to include, fluid flow pattern across the manifold, electrochemical reactions within the cell, and stress profile across the cell and stack.

The results were used in conjunction with correlation chains to establish an optimal design. A new roof for the DFD main chart is proposed to incorporate mathematical models into the design process and arrive at a mathematically optimised solution.

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DECLARATION

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NOMENCLATURE

ρ	Fluid density
u	Fluid velocity vector
t	Time
B	Body force
σ	Stress tensor
h	Enthalpy
λ l	Thermal conductivity
p	Pressure
δ	Kronecker delta
μ	Coefficient of dynamic viscosity
μ'	Second coefficient of viscosity
S_{ij}	Strain rate tensor
K	Coefficient of bulk viscosity

e	Efficiency
T_l	low temperature heat source
T_h	High temperature heat source
E_r	Nernest potential
R	Gas constant
R_{es}	Ohmic resistance
T	Temperature
η	Number of equivalents
F	Faraday constant
E^o	Reversible voltage
ΔG	Standard Gibb's free energy change
P_{H2}	Hydrogen partial pressure
P_{O2}	Oxygen partial pressure
P_{H2O}	Water partial pressure
ΔH	Thange in enthalpy

I	Current across the cell
m	Mass flow rate
A	Active surface area
U	Overall heat transfer coefficient
C_p	Specific heat
V	Cell voltage
$\frac{df}{dt}$	Rate of fuel consumption
E	Young’s modulus
D	Modulus of rigidity
T	Thickness
ν	Poisson’s ratio

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CHAPTER-1
INTRODUCTION

1.1- FUEL CELL TECHNOLOGY

Fuel cells have long been proposed as a clean technology power generating devices. A lot of research and development activity have taken place to bring this technology towards commercialisation to replace conventional power generating devices like the heat engine or gas turbines.

Despite the numerous possible applications of fuel cell systems and despite the impressive advantages and superiority of fuel cells over other power generators, the only application that has passed beyond strictly experimental stage is the supply of electrical power in space vehicles. The reasons for this are apparent from economic considerations and engineering design problems. To date, the huge cost associated with the materials and manufacturing process remains to be the stumbling block. The success of such a revolutionary technology will depend on how much research and development can reduce the cost by, and to what extent the environmental considerations will force us to cover that extra cost for the sake of cleaner environment.

One area researchers have concentrated over the years is, finding cheaper replacement materials for the cell components. Only limited noble materials are suitable for use as fuel cell components due to the mechanical and electrochemical requirements. Nevertheless, we have come a long way in achieving suitable materials and fabrication techniques. One other area that needs exploration is the design strategy employed in the fuel cell development itself. This is the subject matter of this project.

1.2- THE SOFC DESIGN

Several designs of the SOFC have been proposed and developed. Research in Europe has concentrated on the planar design, which is thought to be superior due to its low cost of manufacture. There are also several types of planar SOFC. Coatings of electrodes and electrolyte on a porous substrate, self supporting electrolyte coated with anode and cathode on either side, and self supporting electrodes. The best developed is the self supporting electrolyte. In this SOFC design, electrodes are sprayed or printed on either side of the dense, bulk Zirconia electrolyte to form a sandwich and sintered at high temperatures.

The planar SOFC is an emerging technology: the largest cell built to date has an electrical output of 10kW. Cells have been designed from electrochemical considerations and mechanical design problems have largely been solved by trial and error. Since the mechanical and electrochemical requirements of a SOFC are often in a direct conflict, It is important to find an optimisation strategy that would make a mathematically optimised solution easier to find.

Other SOFC designs include the Westighouse sealless tubular design, monolitic design, and segmented cells in series both cylindrical as well as conical cells. Each of the designs has its advantages and disadvantages over the other cell configurations. The tubular design is the most developed of them all. Its configuration avoids the need for compressive seals, which have proved to be the source of mechanical failure. The cost of fabrication of these cells however is more expensive than planar cells. The segmented cells in series configuration has an advantage in that no support tube is used there by increasing the power per weight ratio and avoiding diffusion and transport problems due to the support material.

This thesis has the broad aim of considering and comparing all the proposed designs in order to achieve a cost effective and mathematically optimised SOFC design. To this end, Design Function Deployment along with Taguchi method of experimentation and mathematical models are employed as design tools.

1.3- DESIGN METHODOLOGY

Design function deployment (DFD) as a design methodology has been developed by Sivaloganathan et al [116] as an extension of the quality function deployment (QFD). In DFD, the definition of a customer includes everyone who requires something out of the design process. QFD emphasises in maximising product quality and tends to ignore engineering science, mathematical optimisation and Taguchi experimentation. DFD is developed to pay more attention to qualitative design and optimisation. Atherton [11] identified parameter selection to be a particularly difficult activity common to QFD and states that identifying parameters and their relationship with the quality characteristics could be done by incorporating engineering science into the formal QFD/DFD design process. By identifying an optimisation strategy linked to the DFD, one could build a complete design methodology.

Atherton argues that the triangular roof of the DFD chart has benefits that are linked to optimisation. Ignoring the correlations between parameters and treating the corresponding parameters as independent can be a source of problems if their target values are changed without assessing the corresponding effect for the correlated parameters. Defining the dependent and independent factors in a relationship is useful information, particularly for redesign, which should be recorded in the roof.

To this end, Atherton [11] proposed a square replacement for the roof of the DFD chart and argues that this dramatically reduces the total solution space, which has to be searched, for two aspects of the design problem.

a) The procedural domain – which includes all design requirements, some of which can not be measured or values assigned to them, which are recorded at a general level in DFD.
b) The physical domain – which can be quantified. Once the independent factors are set the others must follow from physical laws.

Atherton did not test the proposal with a fully worked case study involving complex mathematical equations that call for trade-offs. In this project, the design methodology is tested in the design of a solid oxide fuel cell, which is a complex design problem due to the inherent conflicts between mechanical and electrochemical requirements. Using mechanical reliability, electrochemical performance, and lowering cost, as the quality objectives, highlights the interdependence that often exists between system responses where trade-off has to be made.

1.4- AIMS AND OBJECTIVES

The aim of this project is to design a solid oxide fuel cell using a DFD methodology in order to arrive at a mathematically optimised solution. The design methodology should make it easy to identify the trade-offs and conflicts inherent in fuel cells design and to identify the design rules. Optimum fuel cell design is a compromise between conflicting mechanical and electrical requirements. The design methodology should provide a clear optimisation strategy and optimisation calculations based on the governing equations.

By employing the design methodology, the aim is to reduce the cost associated with the development and fabrication of the solid oxide fuel cell, if possible. Reducing the cost of fabrication of the cell components would certainly see the solid oxide fuel cell technology get closed to commercial reality.

1.5- FINDINGS AND NOVELTY

a) Use of Taguchi methods to find a cost effective manufacturing method for SOFC experimentally.
b) Development of computer programs using engineering principles related to the detailed design of SOFC.
c) Use of DFD in general and correlation chains in particular to develop a conceptual design for a new SOFC – the combined cell.

1.6- THE ROLE OF MODELLING

Through out the design process, design is an abstract: the physical artefact does not exist, so until it is built or manufactured there needs to be some models of the design for those involved to evaluate, manipulate and refine.
Models of the design are used for a variety of purposes. At the most basic level, they are used by the designer to record and manipulate ideas, and to provide a basis for the evaluation of the design. When there are many people involved, as is the case in most design problems, the models have a major role to play in the communication of the design between participants in the process, and to those involved in the manufacture, development and subsequent use of the product. More importantly, however, models are used in getting the design right the first time round. This saves a lot of development time and wastage in trial and error approach.

Computer aided design (CAD) is traditionally understood to be the use of computers to automate or assist in such tasks as the production of drawings or diagrams and the generation of lists of parts in the design. In its advanced level, however, CAD and modelling provides new techniques, which give the designer enhanced facilities to assist in the design process. The driving force behind the provisions of computer assistance for conventional modelling techniques has been the desire to improve the productivity of the designer by the automation of the more repetitive and tedious aspects of design, and also to improve the precision of the design models.

In this project, electrochemical model, fluid flow model and stress analysis are used to evaluate the performance of the fuel cell at the design stage. These models are incorporated into the design process to achieve the optimum parameters for an optimum performance. The stages where each mathematical model is used are identified and a clear problem solving strategy outlined.

1.7- DESIGN ACTIVITY AND CONCURRENT ENGINEERING

In traditional design activity, the design organisation passes its requirements to the machine shop production engineering function in the form of technical drawings. The drawings are interpreted by the production engineers, who draw up process plans using their own practical experience with reference to the former plans for similar parts made in the past. Typically, the production engineers are highly skilled machinists, who have amassed considerable practical knowledge while working in the shop floor environment. The experience of production engineers is enhanced by practical cause and effect learning: unfortunately, no formal record of what has been learnt is kept. DFD have been proposed as a design methodology [73] to record all relevant data and past experience in the design process, which enables future retrieval easy, thus is chosen to be used in this project.

The purpose of knowledge acquisition phase is to identify the design-related causes of problems in the manufacturing environment to steer analytical studies of numerical information and to provide guidance for designers. This was seen to involve production engineer's knowledge of what constituted manufacturing problems, conducting research into solutions and applying those solutions in the context of the design process.

- The process of concurrent design of a material to achieve a specified target performance employing process that ensure product quality and manufacturing effectiveness is a challenging goal. Nevertheless, it holds considerable promise in reducing the technology development times.
- The concurrent design of materials, products, and process that can effectively meet customer requirements is a challenge. It is especially difficult when new technology is required in order to achieve a solution. In such a case, the technology development time can be lengthy which in itself can diminish the value of the result to the customer. Long development times are also costly and increase probability of encountering additional changes in requirements by the customer.

In this project, a Taguchi type statistical experimentation is used to identify an optimum product and process design. This includes identifying the factors that can cause a difference on the product's performance and determine optimum parameter values to improve the quality of the product at minimum cost. Fabrication of the electrolyte material is the main focus as the other cell components are built around it. The cathode, anode and interconnect are designed to be compatible with the electrolyte.

CHAPTER-2

FUEL CELLS - LITERATURE REVIEW

2.1- INTRODUCTION

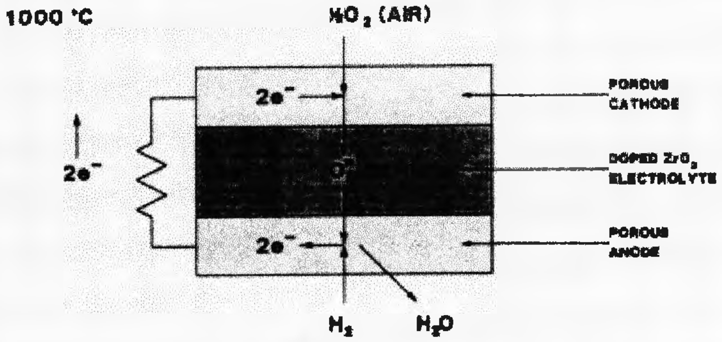
A fuel cell is an energy conversion device that generates electricity by electrochemically combining fuel and oxidant gases across an ionic conducting oxide without combustion as an intermediate step. Direct conversion of fuel energy to electricity is the key characteristic of a fuel cell operation. In conventional thermal power systems, the chemical energy of fuel is transformed first to thermal energy, then to mechanical energy, and finally to electrical energy. The efficiency of the thermal-to-mechanical and mechanical-to-electrical energy conversions is subject to Carnot limitations. The Carnot efficiency of a combustion type system operated between high temperature (T_h) and low temperature (T_l) heat sources is given as [70]:

$$e = 1 - \frac{T_l}{T_h} \qquad [2\text{-}1]$$

Which implies the higher the T_h the better the efficiency. However, there is a practical limit on efficiency, as material stability will limit T_h. The operation of a fuel cell, on the other hand, is not Carnot limited. Thus much higher efficiency (theoretically 80%) can be achieved from a fuel cell system depending on the rate of reaction and loss heat recovery (bottoming cycle) on high temperature fuel cells.In addition to the superior efficiency they posses, fuel cells are inherently clean and are uniquely able to address the issues of environmental degradation. Now market experience is showing that the technology provides a range of critical benefits that no other single power generation technology can match. Among the several emerging environmental issues over the last decade, the level of pollution associated with motor vehicles has been one of the more prominent. In America, Japan and Europe, governments have adopted a strategy that supports alternative models of transportation in order to improve air quality. Fuelled with hydrogen, fuel cells produce no pollutant emissions. Even if fuelled with natural gas as a source of hydrogen, emissions are negligible: 0.45 ppm NO_x, 2 ppm CO, 4ppm HC, which are orders of magnitude much lower than those for conventional combustion generating equipment. Other characteristics that make fuel cell power systems superior include; part load characteristics and response time.

2.2- PRINCIPLE OF OPERATION

The concept of a fuel cell is like that of a battery except that it does not run down. It operates upon a continuous supply of fuel and oxidants. The basic fuel cell structure consists of an electrolyte sandwiched between two electrodes (the anode and the cathode). Fuel is fed to the anode, undergoes an oxidation reaction, and releases electrons to the external circuit. Oxidant is fed to the cathode, accepts electrons from the external circuit, and undergoes a reduction reaction. The electron flow (from the anode to the cathode) produces direct-current electricity. The solid electrolyte conducts ions between the two electrodes.



$$\begin{array}{rlll} \text{CATHODE:} & \tfrac{1}{2}O_2 + 2e^- & \longrightarrow & O^{=} \\ \text{ANODE:} & H_2 + O^{=} & \longrightarrow & H_2O + 2e^- \\ \hline \text{CELL:} & H_2 + \tfrac{1}{2}O_2 & \longrightarrow & H_2O \\ & (CO + \tfrac{1}{2}O_2 & \longrightarrow & CO_2) \end{array}$$

FIG. 2-1 Principle of cell operation

The process is in fact the reverse of electrolysis. It is an isothermal process that involves the conversion of the Gibb's free energy of reaction to electricity. Electrochemical reaction takes place at each electrode:

At the anode,

$$H_2(g) \rightarrow 2H^+ + 2e^-,$$

And at the cathode,

$$2H^+ + \frac{1}{2} O_2(g) + 2e^- \rightarrow H_2O$$

The ions are transferred from the anode to the cathode via the electrolyte, and the electrons via an external load circuit. The overall reaction is therefore:

$$H_2(g) + \frac{1}{2} O_2 (g) \rightarrow H_2O(g) + \text{dc electricity} + \text{heat}$$

2.3- HISTORICAL DEVELOPMENT OF A FUEL CELL

The fuel cell is certainly not a recent invention. In 1802, Sir Humphery Davy reported the construction of a simple cell whose reaction seemed to be

$$C + O_2 \rightarrow CO_2$$

He was able to give himself a feeble electric shock from a battery of such devices [91]. A more obvious fuel cell was that demonstrated in 1839 by sir William Grove, who succeeded in reversing a conventional electrolysis experiment where water (H_2O) was broken down into hydrogen and oxygen by passing an electric current between two platinum electrodes immersed in sulphuric acid producing an electric current by supplying gaseous hydrogen and oxygen. In fact, by using a battery of twenty-six cells he was able to produce enough current to decompose water by electrolysis in yet another platinum -sulphuric acid system. It is interesting to note that Grove, from the very first, realised the essential problem of a working fuel cell would be the difficulty of getting enough reaction to occur at the electrodes for high currents to be taken from the system [79]. This still is a significant problem today. The first use of the name FUEL CELL seems to have been in 1889 by Mond and Langer who, using a similar contrivance to Grove, obtained current densities of about $0.2Acm^{-2}$ which compares quite favourable with modern experience [95]. However, about this time was developed the dynamo, a device for converting mechanical work into electrical energy and the success of this invention caused interest in the fuel cells to lapse for almost sixty years.

Since its discovery, the fuel cell has had a rather chequered history. Development of the Alkaline fuel cell by Bacon in England, starting in the 1930s, resulted in the first practical fuel cell. This was then taken up by Pratt and Whitney for the US space programme and the first real use of the fuel cell was demonstrated in the Apollo moon voyage [42]. Indeed, without the fuel cell, man's first journey to the moon would not have been possible.

Ceramic fuel cells came much later and began with Nernest's discovery of solid-oxide electrolyte in 1899 and the operation of the first ceramic fuel cell at $1000^{o}c$. Nernest [102] discovered solid oxygen-ion conductors when he invented the so-called glower in the end of the 19th century. Nernest proposed to use solid compositions such as ZrO_2 with 15%wt Y_2O_3 addition as a glower to replace carbon filaments in electric lamps. The Nernest glower was operated for hundreds of hours on direct current, though electrolysis was found to occur. It was explained that any loss oxygen liberated at the anode was balanced by an equal amount of oxygen taken into the glower at the cathode [95]. This phenomenon was the reverse of fuel cell operation.

In 1937 Baur and Preis demonstrated the operation of the first ceramic fuel cell [17]. They used mainly ZrO_2 based ionic conductors as an electrolyte, with iron or carbon as the anode and Fe_3O_4 as the cathode. Nernest potential (voltages) between 1.1 and 1.2 V at $1000^{o}c$ were observed. Baur and Preis constructed the first solid oxide fuel cell, with hydrogen or CO as the fuel. A voltage of 0.8 V per cell was achieved.

Much effort was devoted in the 1960s and early 1970s to developing the concept for terrestrial power generation. However, as workers become more aware of the considerable problems in making cost-effective power plant, so the projects were stopped one by one. In a few years only a handful of enthusiasts were left working in the field, and development continued mainly in the United States.

By the mid-1980s improvements in the fuel cell performance, together with a growing concern for the effect of fossil fuel usage on the environment, led to renewed interest world-wide. The reasons are well known. Fuel cells are more efficient compared to conventional power generators and produce less CO_2 per unit of electric power generated. They also produce negligible emissions of SO_x and NO_x.

The most highly developed type of fuel cell at the present time is the phosphoric acid fuel cell (PAFC). The American technology has been developed in Japan to the stage where a number of 50kw on-site power generation units, designed to supply heat and power to offices and factories, are in operation. International fuel cells (IFC) are now also selling their first 200kw natural gas fuelled packages through out the US and Europe. On a large scale, an 11 MW demonstration project run by Tokyo Electric Power Company, equivalent to a small power station, has been in operation [28].

The more efficient molten carbonate and solid oxide cells have reached prototype stage with units of 100kw and 25kw respectively. Plans for commercialising the molten carbonate cell are now advanced in the USA and Europe, whilst development of the solid oxide cell is progressing rapidly in Europe, Japan and the USA. Other cell types such as Alkaline and solid polymer have been demonstrated at sizes of a few kilowatts for remote power generation, transport and marine applications [42].

Initial development work on practical ceramic fuel cells began in the early 1960s. The cell configuration in this time period was either a flat plate or a segmented cell in series designs. These designs used very thick electrolytes, thus suffering significant internal resistance losses. This led to the introduction of thin walled cells that are deposited on a porous support.

In 1980 the seal less tubular design was proposed. Development of fuel cells based on this configuration is still going on. The Westinghouse science and technology centre [132] is the leader in this type of solid oxide fuel cell configuration. A $143 million, 5-year development effort is underway aiming at moving the 21st century technology to the threshold of commercial use. Commercialisation of the Westinghouse concept could offer a new approach for generating power in the United States and world wide. It could create a new solid-state manufacturing industry, employing skilled workers in designing and fabricating power technologies for tomorrow's energy needs.

In the UK, the Government announced a support for fuel cell research programme early in 1992, which focuses on the solid oxide fuel cells [42]. The objectives are to provide a framework for fuel cell research and development in the UK, to evaluate the technical and economic prospects for advanced fuel cell systems, and to accelerate the development of economically attractive advanced fuel cell systems for application in the UK.

2.4- TYPES OF FUEL CELLS

Fuel cells can be classified in many different ways, as there are vast number of variables among the fuel cell systems. These include types of fuel and electrolyte, operating temperature, primary and regenerative systems, and direct or indirect systems. The most common way of classifying fuel cell is the type of electrolyte employed. This section presents an overview of fuel cell technology based on the type of electrolyte.

2.4.1- ALKALINE FUEL CELL

Potassium hydroxide, which is the most conducting of all alkaline hydroxides, has always been the electrolyte of choice for this type of fuel cell. The hydroxyl ions are the conducting species in the electrolyte. Though water is produced at the anode, there is some migration of water to the cathode, and thus, product water exits the cell from the anode (about 2/3) and the cathode (about 1/3).

The unique advantage of an alkaline electrolyte over an acid one for a fuel cell is that noble metal electrocatalysts are not necessary for the former. In addition, even with the non-noble metal or oxide electrocatalysts, the oxygen electrode performance is extremely good. Alkaline fuel cells generally operate at around 60 – 80°c. The low operating temperature (less than 100°c) fuel cells pose difficulty in the product water and heat removal methods.

The Alkaline fuel cell system, using pure H_2 and O_2 as reactants, has established its space application. This system coupled with an alkaline or a solid polymer electrolyte water electrolyser, is a strong contender for NASA's lunar and mars missions, as well as for space stations [28]. The challenges are to develop safe, lightweight methods of gaseous hydrogen storage. Strong hydrogen as a liquid or metal hydride was proposed; but the method was found to be not efficient.

2.4.2- PHOSPHERIC ACID ELECTROLYTE FUEL CELLS (PAFC)

The phosphoric acid fuel cell, which operates at about 200°c, is by far the closest to commercialisation. One can purchase a 200kw co-generation plant from international fuel cells (IFC) in the United States. This unit will run on pipeline natural gas and generate electricity at about 40% compared with 31% for engine based alternatives at the same capacity [28]. NO_x emissions are as low as 2ppm compared with about 2000ppm for a cleaned up reciprocating engine. The down side, however, is that they are twice the price at the present.

Phosphoric acid is the electrolyte of choice for acid electrolyte fuel cells, particularly with hydrogen produced by steam reforming of organic fuels.

The attractive features of phosphoric acid are:

1- Stability in the electrochemical environment at temperatures up to about 225°c;
2- Reasonably good electrolyte conductivity at temperatures above 150°c; and
3- Efficient rejection of product water and waste heat at the operating temperature.

2.4.3- MOLTEN CARBONATE FUEL CELLS (MCFC)

The molten carbonate fuel cell is second generation device in that no fully engineered product exists yet. It offers system efficiencies of 50% or higher and demonstration units at over 100kw have been run. Operation at 650°c makes internal forming possible, simplifying the plant and improving performance. Major challenges include corrosion resulting from the molten salt environment and the need for CO_2 recycling to retain the carbonate balance. This imposes a performance penalty.

Molten alkali carbonate mixture, retained in porous lithium aluminate matrix, is used as the electrolyte. Since the MCFC operates at about 650°c, a power plant with cell stacks of this type has several favourable characteristics for utility power generation:

1- polarisation losses are reduced to such an extent that it does not require expensive catalysts as do low temperature fuel cells, such as PAFC,
2- the operating temperature is high enough to produce high quality waste heat.

Plans are underway to design and construct MCFC power plants of megawatt-size capacity for base load and intermediate load power generation and co-generation applications.

2.4.4- THE SOLID OXIDE FUEL CELL

It is well known that solid oxide fuel cells (SOFC) have attracted considerable interest during the past decade as highly effective and environmentally acceptable sources of electrical energy. Among fuel cells it is believed that they can offer the widest potential range of applications and high system efficiency, also achievable by use of waste heat released at high temperature level in co-generation applications and bottoming cycles. Moreover, operating conditions allow the utilisation of fuel with high contents of carbon monoxide.

Current solid oxide fuel cells use an oxygen-ion conductor or a proton conductor as an electrolyte and operate at high temperatures (commonly 1000°c). SOFC are presently under development for a variety of power generation applications. The most advanced SOFC are those based on oxygen-ion conducting stabilised zirconia electrolyte. The conductivity requirement for the electrolyte determines the operating temperature of this SOFC (about 1000°c). The other materials commonly used for this type of SOFC are nickel stabilised zirconia cermet for anodes, doped lanthanum manganite for cathode, and doped lanthanum chromite for interconnects.

SOFC have several distinct advantages over other types of fuel cells. E.g., use of non-precious materials, no liquids involved in the fuel cell, and invariant electrolyte. The use of solid electrolyte eliminates material corrosion and electrolyte management problems. The high operating temperature promotes rapid reaction kinetics and allows reforming of hydrocarbon fuels within the fuel cell (internal reforming). Thus power systems based on solid oxide fuel cells can be simple and are more efficient than many other technologies. Furthermore, because all the components are solid, SOFC can be fabricated in very thin layer, and cell components can be configured into desirable shapes and sizes unachievable in fuel cell systems that has liquid electrolyte. On the other hand, ceramic fuel cells place stringent requirements on materials. Ceramic fabrication processes need to be developed to incorporate the materials into practical stack configurations. At present the key technical challenge is development of suitable materials and fabrication of ceramic structures. Engineering ceramic powders and developing forming and processing methods play a key role in ceramic fuel cell technologies.

This project is concerned in the design of solid oxide fuel cells alone. Cell components and different conceptual designs are explored in detail in the next sections.

2.5- SOLID OXIDE FUEL CELL COMPONENTS

A SOFC single cell consists of an oxide electrolyte sandwiched between an anode and a cathode. Under typical operating conditions (with hydrogen fuel and oxygen oxidant), a single cell produces less than 1 V. Thus practical SOFCs are not operated as single units; rather, they are connected in electrical series to build voltage. A series of cells is referred to as a stack. An interconnect material connects the anode of one cell to the cathode of the next cell in the stack. Each component serves several functions in the fuel cell and must meet certain requirements.

2.5.1- ELECTROLYTE

The main function of the electrolyte material is to conduct ions between the anode and cathode. It carries the ions produced at one electrode to the other to balance the charge from the electron flow and complete electrical circuit in the fuel cell. The electrolyte also serves, as a separating wall between the fuel and oxidant thus must be dense (non-porous) to prevent fuel or oxidant diffusion either way. The ion-conducting electrolyte must also be an electronic insulator; it shouldn't conduct electricity as that may cause a short circuit. Stabilised zirconia (ZrO_2), especially yittra-stabilised, is the most common electrolyte in SOFCs because it possesses an adequate level of oxygen ion conductivity and exhibits desirable stability in both oxidising and reducing atmospheres. ZrO_2, in its pure form, does not serve as a good electrolyte, primarily because its ionic conductivity is too low. At room temperature, ZrO_2 has a monoclinic structure that changes to a tetragonal form above a temperature of 1170°c and to a cubic fluorite structure above 2370°c. The tetragonal monoclinic transformation is associated with large volume change (3% to 5%) (contracts on heating and expansion on cooling). The cubic phase exists up to the melting point of 2680 °c. However, the addition of certain aliovalent oxides mainly yittra (Y_2O_3) stabilises the cubic florite structure of zirconia from room temperature to its melting point and, at the same time, increases its oxygen vacancy concentration. This enhances the ionic conductivity and leads to an extended oxygen partial pressure range of ionic conduction, making stabilised ZrO_2 suitable for use as an electrolyte in SOFCs. This extended oxygen partial pressure range covers the conditions 1 to 10^{18} atm to which a SOFC electrolyte is exposed in the fuel cell during operation.

Yittra stabilised zirconia (YSZ) must be fabricated into fully dense layer for use as a SOFC electrolyte. A common fabrication method is the particulate approach. This involves compaction of YSZ powder into the desired shape and densification at elevated temperature. In general, densification of materials consolidated by the particulate approach is dependent on material and processing factors, such as powder characteristics (reactivity, purity, morphology) particle packing (green density) and processing conditions (temperature, time, atmosphere). Ideally, fine particles with narrow size distribution are desirable because they result in high reactivity and high packing density, which enables a uniform microstructure of the sintered & compacted powder to be achieved.

Development of other materials, especially those possessing sufficient ionic conductivity at intermediate temperatures (600^oc to 800^oc) has received much interest recently. A replacement of YSZ by reduced temperature oxygen-ion conductor would greatly reduce material and fabrication problems. Until that time, YSZ will dominate as the material to be used as an electrolyte of a solid oxide fuel cell.

2.5.2- ANODE

The main function of a SOFC anode is to provide reaction sites for the electrochemical oxidation of the fuel. Thus, the anode material must be stable in the fuel-reducing environment and have sufficient electronic conductivity. Because of the reducing conditions of the fuel gas, metals can be used as SOFC anode materials. Suitable metals can be non-oxidised at the oxidising environment an anode is exposed to and at operating temperature of 1000^oc. These metals are limited mainly to nickel cobalt and noble metals. Nickel is commonly used because of its low cost compared to other metals such as cobalt, platinum and palladium. The anode, unlike electrolyte, has to have adequate porosity to allow diffusion of ions to the reaction site. In its pure form, nickel can not maintain porosity at the working temperature of 1000^oc. The metal is then dispersed on the surface of YSZ support. The support is added to the anode formation in the form of powder or fibre. The functions of the YSZ support in the anode are to support the nickel metal particles, inhibit coarsening of metallic particles at the fuel cell operating temperatures, and provide an anodic thermal expansion coefficient acceptably close to those of the other cell components [100]. Compatibility of thermal expansion coefficient is important as it may cause stress build up or even cracking due to differential expansion. The electrical conductivity of nickel /YSZ cermet is strongly dependent on its nickel content.

Since nickel has higher thermal expansion coefficient than YSZ, there are concerns about thermal expansion mismatch between the anode and electrolyte. As explained above, mismatch in thermal expansion has a detrimental effect during working conditions and/or fabrication. The thermal expansion coefficient of nickel/YSZ cermet increases linearly with the nickel content. This is where trade off is required between conductivity and reduction of thermal expansion coefficient. Various means have been developed to tolerate and minimise the thermal expansion mismatch. Some of these include, improving the fracture toughness of the electrolyte to provide sufficient tolerance of stresses generated by thermal expansion mismatch and/or varying the thickness and thickness ratio of the cell components.

2.5.3- CATHODE

The main function of the cathode is to provide reaction sites for the electrochemical reduction of the oxidant. Thus, the cathode material must be stable in the oxidant oxidising environment and have sufficient electronic conductivity. Because of high operating temperature (1000°c) of the YSZ based SOFC, only noble metals or electronic conducting oxides can be used as cathode material. Noble metals, such as platinum, palladium and silver are unsuitable for practical applications because of excessively high cost. Several doped oxides and mixed oxides have been proposed and investigated. The disadvantages of most of these materials are thermal expansion mismatch and incompatibility with the electrolyte and lack of conductivity. At present, doped lanthanum manganite ($LaMnO_3$) is most commonly used.

$LaMnO_3$ is a p-type perovskite oxide. At high temperatures, the material can have oxygen excess, stoichiometry, or deficiency depending on oxygen partial pressure (the total pressure multiplied by the percentage of oxygen composition in the mixture-air) [100]. For example, at 1200°c, the oxygen stoichiometry of the material ranged from 3.079 to 2.947 under oxygen partial pressures of 1 to 10^{11} atm [94]. In oxidising atmospheres, $LaMnO_3$ has oxygen excess and the amount of excess oxygen varies with temperature. In reducing atmospheres, the material becomes oxygen deficient. Under very reducing conditions, $LaMnO_3$ dissociates into $La2O_3$ and MnO

2.5.4- INTERCONNECT

The main function of the SOFC interconnect is to provide electrical connection between an anode of one cell and a cathode of the next in the electrical series. It also serves as a seal, separating the fuel from the oxidant in the adjoining cells of the stack. Thus, the interconnect material has to be stable in both reducing and oxidising environments, impermeable to gasses to prevent diffusion taking place through the wall, and adequate conductivity to support the electron flow at the operating conditions. It must also posses thermal expansion compatibility with other cell components.

The stringent requirements for the interconnect of a SOFC eliminate all but few oxide systems from consideration. Lanthanum chromite ($LaCrO_3$) is particularly suitable from the standpoint of high electronic conductivity under fuel and oxidant atmospheres, stability in the fuel cell environment and compatibility with other cell components. $LaCrO_3$ is currently the most common material for the interconnect in the SOFC.

2.6- TYPES OF SOLID OXIDE FUEL CELLS

At present, there are four common stack configurations proposed and fabricated for solid oxide fuel cells: sealless tubular design, segmented cell in series design, monolithic design, and flat plate design. The designs differ in the extent of dissipative losses with in the cells, in the manner of sealing between oxidant and fuel channels, in making cell to cell electrical connections in the stack, and in the manufacturing (fabrication) techniques employed.

2.6.1- TUBULAR DESIGN

The sealless tubular design is the most advanced among the several SOFC concepts proposed. In this design, the cell components are configured as thin layers on a closed -one-end tubular support. The tubular concept of the SOFC was first introduced by Rohr [109] at the Westinghouse electric corporation research laboratories. The design used a porous 15% calcia-stabilised zirconia support tube, 1-2 mm thick, on which the cylindrical cermet anodes of individual cells were deposited by filtration and sintered [97]. The anodes were separated by bands of bare support tube, produced by electrochemical etching. After masking, a band of interconnect material was then deposited by EVD over the end of each anode. After further masking, the electrolyte was deposited by EVD in such a way that a cylindrical band of this interconnect material was still exposed. The end of each electrolyte, next to the interconnect was then masked, a porous layer of tin-doped indium oxide was deposited by chemical vapour deposition (CVD). Finally, this layer was impregnated with praseodymium nitrate, which was heated to form a catalytic cathode. The cells were edge connected in series, the current being carried along the length of the anode of one cell to the interconnect, and then along the length of the tin doped indium oxide cathode current collector of the next cell. The whole system was a solid state thin-film version of the bell and spigot structure, bearing the same relationship to it as a printed circuit board does to a soldered electronic device. Indeed, the procedures used were inspired by those in electronics. At 1000°c, maximum power densities of $0.3W/cm^2$ with hydrogen and oxygen and $0.2W/cm^2$ with hydrogen and CO-air were attained with this complex structure of small cells [17,97]. The air electrode and current -collector structure was later abandoned because of the high vapour pressure of indium oxide at 1000°c.

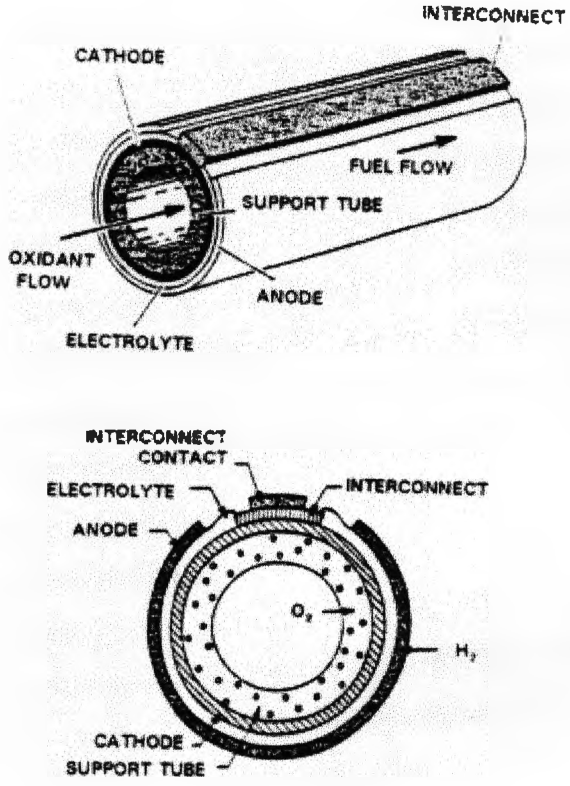


FIG. 2-2. Tubular design configuration

The design was modified at Westinghouse by Isenberg [71], in 1980-82, by turning it inside out so that the anode was external, which allowed a simpler form of current collection in the anode atmosphere by using a nickel felt between the anode of one cell and the interconnect of the next. It uses a closed-end tubular support upon which the cathode, interconnect, electrolyte, and anode are sequentially deposited. Air is fed into the tube via a concentric alumina air injection tube. The air injection tube is integrated with a heat exchanger, to allow maintenance of the correct cell operating temperatures as a function of power output.

As in the original concept, the support tube is made of calcia-stabilised zirconia, which accounts for 50% of the materials cost, because it is much higher than that of the cell itself. It therefore has a significant effect on the specific power densities. An advantage of this design is that the support tube provides a structural support for the cell components so that their structure can be made very thin. This reduces the ohmic losses in the electrolyte layer, but current is collected peripherally in this system, which means the layer thickness cannot be significantly reduced nor can tube diameter be significantly increased. At present, the support tube has a diameter of about 1.5-cm, a wall thickness of 1.5mm, and a porosity of about 50% to allow oxygen to diffuse to the cathode. Its length varies from 30 to 60 cm, and it has an effective surface are of 100-200 cm^2, since the upper (open) part of the tube is inoperative as a fuel cell, serving as a manifold in a ceramic header.

Since the support tube consists of stabilised zirconia, its thermal expansion coefficient matches those of the electrolyte, cathode, anode, and the interconnect. It is fabricated by extruding a cylindrical section, inserting a plug to close one end, and sintering. The porous air electrode is fabricated by filtering a slurry of Sr-doped $LaMnO_3$ powder over the support tube and sintering the composite structure to produce a layer approximately 1 mm thick over the entire cell length. The support tube, with its sintered air electrode structure, is then masked and further processed by deposition of a Mg-doped LaCrO3 interconnect film about 30 microns thick, using electrochemical vapour deposition (EVD). The dense yittra-stabilised zirconia electrolyte film, about 30 microns thick, is then deposited over the tubular assembly by EVD after making the interconnect.

The electrolyte film formed over the air electrode is uniform in thickness and provides a gas tight barrier during the exposure of the cell to the oxidant and the fuel atmosphere. During this stage the pores in the air electrodes are filled with the yittra-stabilised zirconia.

In the second stage of the reaction, electrochemical reduction of oxygen occurs at the air electrode-CVD electrolyte layer interface, and oxide ions pass to the surface of the CVD layer in contact with the mixed chlorides, where they react to give an increased thickness of dense doped oxide and chlorine. In this part of the process, the oxide ion is transported electrochemically, so the technique is thus labelled EVD.

Finally, a porous nickel-zirconia cermet fuel electrode layer with a thickness of about 100 microns is deposited on the electrolyte by the application of nickel powder slurry. This is followed by its impregnation with yittra-stabilised zirconia by EVD. The cells are then checked for gas tightness before electrical testing.

A 400-W SOFC generator was designed and constructed by Westinghouse Electric (USA) and was delivered to Tennessee Valley Authority (USA) in 1986. It was successfully operated for 1760 h [100]. This demonstrator showed the capability of the system for automatic unattended operation. In 1987 two 3-kW systems were built by Westinghouse Electric and installed and tested at Osaka Gas Company and at Tokyo Gas Company with reformed, desulfurized pipeline natural gas as fuel. Both units have met the target specifications of 50% efficiency and also sustained the expected low environmental impact of SOFC [17].

2.6.2- MONOLITHIC DESIGN

The monolithic solid oxide fuel cell (MSOFC), first proposed by Argon National Laboratory [9] in 1983, is a planar cell design in which the ceramic cell components mutually support each other. Thus, no supporting material is used, and all the components are active, allowing enhancement of the specific power density (in terms of both power per volume and power per weight). It is projected that this design may offer power densities of 8.08*10^3 W/kg and 4*10^3kW/m^3, compared with 100W/kg and 140kW/m^3 for the Westinghouse tubular system [132].

MSOFC are still in an early stage of development, and much more research and development is required before the system becomes truly practical.

Fig.2-3 shows a schematic cross section of a MSOFC in a coflow configuration, indicating the component materials

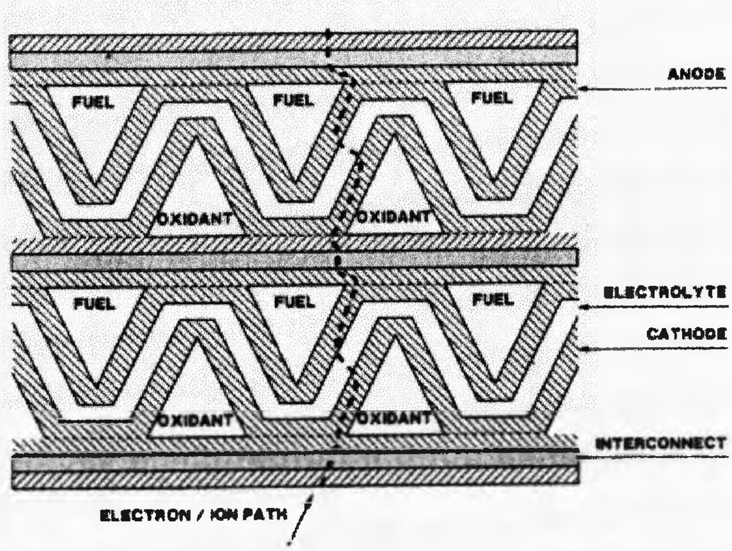


FIG. 2-3. Monolithic cell design configuration

Presently, MSOFCs are fabricated by the following steps:

(1) slurries of electrode, electrolyte and the interconnect material powder are made;

(2) tape-casting or tape-calendering process are used for the production of thin green ceramic layers;

(3) these layers are laminated, corrugated, and stacked;

(4) the electrochemical cell stack is sintered.

Tape casting is a common fabrication process used for forming large area, thin, flat ceramic layers. The process uses slurry of ceramic material dispersed in a dilute solution of organic binders and plasticizers in a suitable solvent. This is spread on a flat surface from a linear hopper perpendicular to the direction of the film to a controlled thickness using the knife-edge of a doctor blade moving with the hopper. The solvents are then allowed to dry, giving a flexible tape containing the ceramic powders and plastic binders, which can be stripped from the casting surface, cut to size, and corrugated before firing. The anode, electrolyte, and cathode layers are fabricated by sequential casting one layer on top of another.

A tape calendering technique, similar to tape casting, can also be used to produce thin, flexible green ceramic layers. In this process, the ceramic powder, binder, and plasticizer are mixed in a high intensity mixer. The friction resulting from the mixing heats the batch to form a plastic mass. This is then calendered into a thin flat tape in a two-roll mill. To fabricate composite tapes, individual tapes are laminated in a second rolling operation. These are corrugated using a two piece mould designed to yield the desired corrugation pitch and amplitude. The tape to be corrugated is laid on the bottom half of the mould, and the top half is lowered to engage the first corrugation. This process is then advanced to the remaining corrugations successively until the entire tape has been formed on the bottom mould. Corrugation has also been carried out by compression moulding. The corrugation step is followed by cutting, then stacking in the proper sequence and orientation to form the fuel cell stack. Following the corrugation process, the laminated layers may be compressed into a honeycomb-like structure. This stack is then sintered at the desired temperature to complete the fabrication process.

2.6.3- PLANAR DESIGN

Whereas the MSOFC is made up of components which are sintered in one piece, planar designs which superficially resemble it are made by building up separately fired components. Planar designs of this type may therefore have the advantage of posing less technological risk than monolithic structures, even though their assembly may be more complex and costly. Planar SOFCs may also have some advantage over tubular designs, particularly in their potential for allowing a higher power density, and simpler, less costly methods of fabrication. They may be regarded as a compromise between tubular and monolithic SOFCs. Planar cells may be more suitable than tubular SOFCs for large scale power plants, because they contain a lower mass of raw materials, reducing cost, and since they are bipolar rather than having edge collection of current, the ohmic resistance of tubular cells will generally be larger than that of the planar cells [17,100]. In addition, large power plants with a tubular design will require a very large number of separate cells and electronic connections, which will increase cost compared with that of plants consisting of a small number of bipolar stacks. Planar cells are being developed at a number of research and development facilities.

Planar cells have normally been fabricated by tape casting. Characteristic methods of preparation have been reported by Iwata [72]. Electrolyte layer slurries were prepared by mixing an organic binder, a solvent, a dispersant, a plasticizer, a homogenizer, and yittra-stabilised zirconia powder in a ball mill. Using the doctor blade method, the slurry was cast into tapes of thickness between 500 and 700 microns. These tapes were then cut into the sizes required. The green samples were first burnt out at 350°c to remove the organic compounds, and then calcined at 1500c for about 2h. The final samples were 300-500 microns thick.

To form the anode layer, ethanol was added to mixture of nickel oxide and yittra-stabilised zirconia, which was ball-milled and calcined at 1500°c for 2h to give a uniform powder. Ethanol slurries of this crushed Ni (35% vol)-yittra-stabilised zirconia cermet powder were then prepared. The slurry was then coated on the electrolyte layer and sintered at 1500°c for 2h. The final thickness of the anode layer was about 150-200 microns [96].

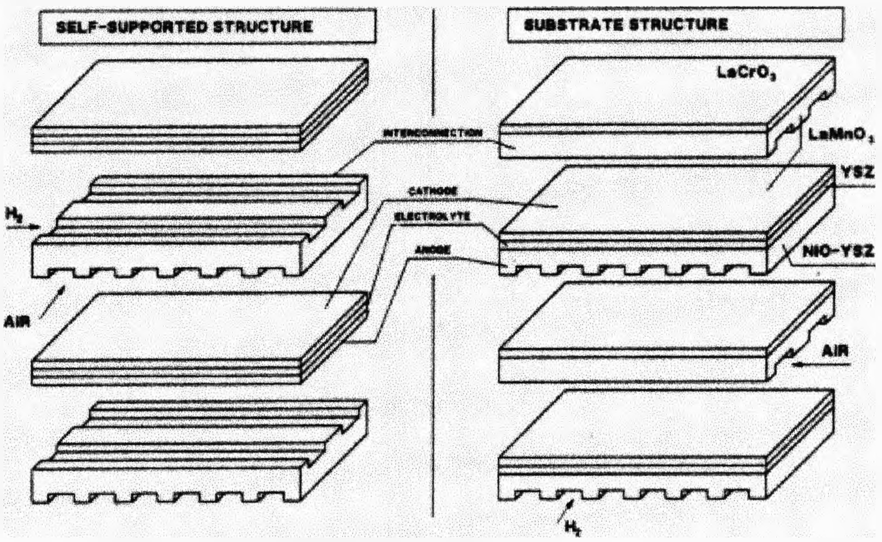


FIG. 2-4. Planar cell design configuration

For the cathode layer, lanthanum oxide, strontium carbonate, and manganese carbonate powders were mixed in proportion to give the composition $(La_{0.7}Sr_{0.3})_{0.9}MnO_3$ with ethanol, ball milled and calcined at 1000°c for 2h . Lanthanum strontium manganite slurries were then prepared from the crushed powders. These slurries were coated on the electrolyte plates and calcined at 950°c for 2h. Slurry coating was also carried out by a screen-printing process. The final thickness of the cathode layer was between 150-200 microns. The interconnect material (Sr-doped lanthanum chromite) can be sintered in air and usually tape-casted and fired separately in a reducing atmosphere and attached to the cell for planar SOFCs.

2.6.4- SEGMENTED CELL-IN-SERIES DESIGN

The segmented cell in series design consists of segmented cells connected in electrical and gas flow series. The cells are either arranged as a thin banded structure on a porous support tube (banded cell configuration) or fitted one into the other to form a tubular self supporting structure (bell-and-spigot configuration). The interconnect provides sealing (and electrical contact) between the anode of one cell and the cathode of the next cell. In this design, the fuel flows from one cell to the next inside the tubular stack of cells and the oxidant flows outside. In the banded cell configuration, where the support tube is used, cells can be made with component thickness on the order of 100 to 250 microns. In the bell and spigot configuration, individual cells form into short cylinders of about 1.5 cm in diameter. The cells are about 0.3mm thick to provide structural support.

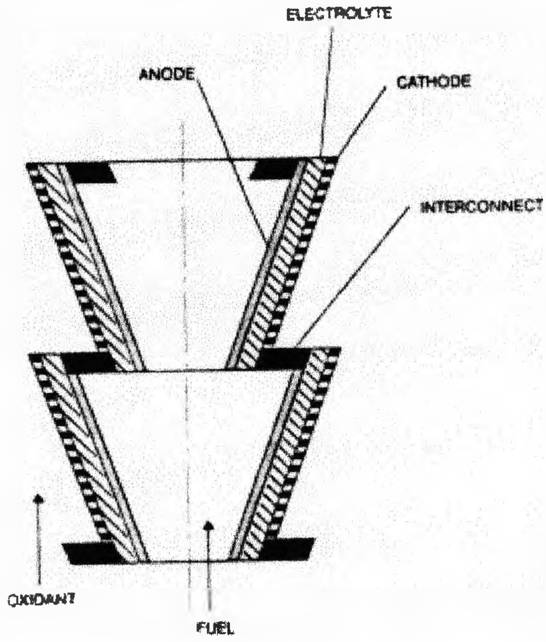


FIG. 2-5. Segmented-cell-in-series design configuration

The segmented cell in series design offers the advantage of improved efficiency. Cells in gas flow series have less power wasted in resistance losses because the first cell in series has higher output voltage. For example, four or five cells in fuel flow series can generate about 10% more power than a single cell of the same total active area [96]. The benefit of adding still more cells diminishes rapidly above five or six cells in fuel flow series. Like the sealless tubular design, the thick support tube in this design restricts gas transport, thus limiting cell performance. In the case of bell and spigot configuration, the self-supporting electrolyte reduces the losses arising from gas transport but can significantly increase the resistive losses. Cell internal resistance is an important consideration in this design. The cell length is kept short to minimise the path for current in the electrodes. Gas tight seals are required for the segmented-cell-in series design. Fuel and oxidant must be separated by a seal on both ends of a stack. In addition, gas tight seals must be maintained between each cell at interconnecting areas.

At present, the cell layers of the banded cell configuration are made by a process based on plasma and flame-spraying methods. Plasma spraying is a process in which the desired coating material in powder form is heated to above its melting point while being accelerated by a carrier gas stream through an electric arc. The molten powder is directed at the substrate, and on impact, forms a coating on the substrate surface.

The fabrication of the components on the support tube is as follows. Gas tight Al_2O_3 layers are first applied on the tube by plasma spraying. The function of these thin Al_2O_3 layers is to provide sealing at interconnecting areas. During spraying, the support tube rotates around its axis while the spray gun traverses along the support tube axis. The anode is coated on the support tube by an acetylene-flame-spraying process. The electrolyte is plasma sprayed on the anode after appropriate masking. A minimum thickness of about 100microns is required to achieve gastightness with out pinholes [97]. The gas tightness of the electrolyte has been improved by applying low-pressure plasma spraying recently, a coating technique based on a CO_2 laser have been developed for making electrolyte layers. The interconnect is fabricated by plasma spraying. The interconnects at the end of the support tube are covered with Al_2O_3 coating to prevent oxidation during cell operation. The cathode is deposited on the electrolyte and interconnect layers by acetylene flame spraying. During the spraying process, the crystalline structure of the cobaltite cathode can be destroyed; however, the structure is recovered by firing at 1100°c for several hours in air.

For the bell and spigot SOFC, self-supporting electrolytes are fabricated by axial pressing. Diffusion welding is used to make the interconnection seal between electrolyte cylinders. The electrodes are applied by slurry coating.

At present, development work on the segmented-cell-in series design has been focused on the banded cell configuration. Six-, twelve-And fifteen-cell tubes have been fabricated. Cell performance of 0.65 V at 200 mA/cm^2 and 80% fuel utilisation has been achieved, and stacks have been tested for more than 5000 h. A 1-kW module containing 48 tubes has been constructed and operated. A power output of 1.3 kW at 56% fuel utilisation has been achieved [17].

2.7- MATHEMATICAL ANALYSIS OF FUEL CELLS

Fuel cells have been investigated and developed, mainly because of high energy conversion efficiency. These researches have been concentrated on the development of the electrode materials, the electrolyte material and the construction of the cells in general. Recently, mathematical modelling has been taken as an important tool for the design of solid oxide fuel cells and for the prediction of their operating performances. Some work has been done in this field with increasing interest during the last few years. These include: thermodynamic models with internal and/or external methane reforming, electrochemical models, thermal models, and a prediction of an on design and off-design performance for a solid oxide fuel cell power module.

Demin and Alderucci [40] have done an extensive thermodynamic analysis on different versions of external reforming of methane for solid oxide fuel cells. Their work included comparing steam reforming, partial oxidation, and exhaust gas. They used an electrochemical generator, where the reactions involved in the reformer, in the fuel cell, and in the exhaust gas section were separately analysed. Equilibrium calculations were performed in the temperature range of

1000 - 1400 k assuming different oxidised /reduced component ratios at the inlet and outlet of the electrochemical section. Their results pointed out that the most efficient way to feed a SOFC to be by exhaust gas reforming.

It has become evident, however, that internal reforming of methane is crucial point to be considered since the cooling effect of the endothermal reforming reaction strongly affects the operating conditions of the cell stack. The steam necessary for the reforming reaction can be advantageously taken from the fuel cell system itself. Since double the amount of H_2O is electrochemically produced than is needed for the reforming process, partial feed back of the anode gas is recommended to minimise engineering expenses.

Eguchi [48], in 1995, conducted an experimental analysis of internal reforming activity during power generation. In the experiment, a methane and steam mixture (H_2O / CH_4) was supplied to a tubular fuel cell fabricated by the slip casting process. A gas phase analysis was carried out during the measurement of the fuel cell experiment. Methane conversion and formation rate of H_2 at the open circuit condition increased with increasing temperature. This increase was mainly due to enhancement of the rate constant of the reaction and partially that of the equilibrium conversion. The selectivity to CO_2 was lowered and the CO formation became dominant at high temperatures. The effect of flow rate of the reactant gas was measured at 20% CH_4 and 40% H_2O. The open circuit voltage and the voltage-current density characteristics were unchanged with the overall flow rate of the reaction gas. The methane conversion at the open circuit condition decreased as the overall flow rate increased, since a large amount of methane was supplied to the system.

Internal reforming is now seen as one of the main advantages of the SOFC over other types of fuel cells. It has been found to reform methane internally to some degree; this apparently occurs at the Ni/ZrO_2 cermet anode. This internal reforming not only makes for a simpler system, but results in a higher cell efficiency due to the decreased energy loss associated with the transfer of heat to an external reformer. Experimental results performed by Lee [85] have shown that the reforming reaction can be written as:

$$rCH_4 = k\,(pCH_4)(pH_2O)^{-1.25} \qquad [2\text{-}2]$$

Where pCH_4 and pH_2O are the partial pressures of methane and steam, respectively. The value k is the rate of reaction and can be written as:

$$k = k_o\, e^{(-E/RT)} \qquad [2\text{-}3]$$

Where k_o is the frequency factor and E is the activation energy.

Internal reforming, however, has its own shortcomings. The problem that arises is that the reforming reaction is highly endothermic and can result in a 'cold' spot in the cell. This could degrade performance or result in excessive thermal stresses. Bessette [14] outlined the effect of internal methane reforming on the temperature profiles. Most methane is known to be reformed within the first 10cm of the cell length due to the high rate of chemical kinetics encountered at 1000°c. For methane, the enthalpy of reformation is very high, around 200 KJ/mol. Combining these two effects, even low percentages of methane, from 5 to 20%, lead to severe decrease in temperature at inlet of the fuel stream. For the 5% reforming case, there is little effect on the temperature and inlet profile is what would be expected. The results obtained from Bessette's calculations agree with Westinghouse experimental data.

Bessette [15] presented a mathematical model of a tubular solid oxide fuel cell. In his work, the complete electrochemical and thermal factors were accounted for in a rigorous manner. According to N.F. Bessete, the two possible overall reactions occurring in the sealless tubular SOFC are:

$$H_2 + \frac{1}{2} O_2 \rightarrow H_2O$$

and

$$CO + \frac{1}{2} O_2 \rightarrow CO_2$$

depending on whether only hydrogen or both hydrogen and carbon monoxide can react. Here both activation polarization and concentration polarization are accounted for quantitatively. Bessette determined all required parameters from independent sources; non were fit from performance data. To verify accuracy of his work, model predictions were compared with single cell test data from Westinghouse. Agreement with electrochemical and thermal results were with in 5%.

Ahmed [5] whose work was based on a cross flow monolithic solid oxide fuel cell has also developed a model to simulate the electrochemistry and thermal hydraulics of the cell. Unlike bessette's work, losses of activation and concentration polarization are not accounted for quantitatively . An assumption was made on the cell operating voltage taking the losses into consideration.

The current generated was then evaluated as;

$$I = \frac{Er - V}{Res} \qquad [2\text{-}4]$$

Where, *Er* is nernest potential

*R*es is ohmic resistance

V assumed cell operating voltage.

Kanamura [77] concentrated on the temperature and thermal stress distributions in a cell. He used finite element method inorder to determine guidelines for the selection of cell materials for both planar and tubular fuel cell configurations. His calculations indicated that the heat generated from the entropy change of cathode reaction has significant effect on the temperature distribution in tubular solid oxide fuel cells. For planar SOFC model, the largest stress generated were in the region of the cathode material.

Most of these mathematical models tend to concentrate on a single cell performance. Most researchers have chosen simply to assume that the performance of multiple cells is just a linear extension of a single cell performance. Bessette [15] seems to disagree. He pointed out that, inorder to assess accurately the performance of a solid oxide fuel cell system, the characteristics for power, or 'stack', module must be known. These results cannot be obtained simply by scaling up a single cell model because system performance is not linearly proportional. In a stack, most cells not only produce current but also must carry current generated by other cells. Likewise, the thermal enertia of the stack system and enclosure leads to heat transfer calculation in a single cell model.

A mathematical simulation is helpful in determining the cell's performance characteristics. Such a simulation can be used to determine the effect of varying the design and operating parameters on the power generated, fuel conversion efficiency, and maximum cell temperatures reached. In addition, such simulations can provide answers to questions such as how thin the electrolyte layer needs to be, or what the air and fuel flow rates must be to avoid excessive temperatures and/or pressure drops. Thus, mathematical modelling offers the potential to direct the technology development, test the significance of various design features and the effectiveness of the developments in materials or fabrication procedures, and select optimum operating conditions from the feasible set of process parameters.

2.8- THERMODYNAMIC PRINCIPLES OF SOFCs

The operation of SOFCs based on a hydrogen fuel and oxygen involves the oxidation and reduction of oxygen at the electrodes. Nernest established the relation of the reversible cell voltage and the electrode reactions. The potential (voltage) at the cell is given as [67,96]:

$$E_r = E^o + \frac{RT}{2nF} LnPO_2 + \frac{RT}{nF} Ln \frac{pH_2}{PH_2O} \qquad [2\text{-}5]$$

Which can be simplified as

$$E_r = E^o + \frac{RT}{nF} Ln\left(\frac{PH_2 PO_2{}^{1/2}}{PH_2O} \right) \qquad [2\text{-}6]$$

Where E^o is the reversible voltage at the standard state. At a standard state E_r equals E^o and the following equation is established for every fuel:

$$E^o = \frac{-\Delta G^o}{nF} = \frac{-\Delta H^o - T\Delta S}{nF} \qquad [2\text{-}7]$$

Where $-\Delta G^o$ is the standard Gibb's free energy change of combustion reaction of the fuel, ΔH^o the standard enthalpy change, ΔS the standard entropy change, and n the number of moles of oxygen required to oxidise one mole of fuel multiplied by four. The maximum energy obtained in this case is given by $-\Delta G^o$, and the ideal thermodynamic efficiency (e_t) is represented by:

$$e_t = \frac{\Delta G^o}{\Delta H^o} \qquad [2\text{-}8]$$

The operating cell voltage is, however, always less than the reversible voltage (Nernest potential). As the current is drawn from the fuel cell, the cell voltage falls, due to various losses. The reduction in the cell voltage under current load depends on current density and several factors such as temperature, gas flow rate and composition, and cell material. The difference between the operating cell voltage and the expected reversible voltage is termed polarisation or overpotential. Three types of polarisation are significant in high temperature fuel cells: activation polarisation, concentration polarisation, and ohmic polarisation. Polarisation can not be eliminated but can be minimised by material modification and cell design.

The increase in operating temperature, for example, reduces cell polarisation by enhancing mass transfer, increased reaction rate and lower material resistance. Increase in operating temperature, on the other hand, may limit material choice and accelerate material-related problems such as interface delamination and degradation. An increase in the operating pressure improves fuel cell performance because of increased reactant partial pressure and increased mass transport rate. On the other hand, increase in pressure also imposes limits on material selection and causes other problems or concerns such as integrity of the gas seal and cell structure.

(a) Activation polarisation: chemical reactions including electrochemical reactions involve an energy barrier that must be overcome by the reacting species. This energy barrier, called the activation energy, results in activation polarisation may be regarded as the extra potential necessary to reduce the energy barrier of the rate-determining step of the reaction to value such that the electrode reaction proceeds at a desired rate. Activation polarisation is due to one or more slow rate-determining steps in the electrode reaction. The slow step could be related to adsorption of reactant onto the surface of the electrode, election transfer, or any other step in the reaction. The electrode reaction rate is a function of temperature, pressure, and electrode material. At high temperatures as in the case of SOFC, reaction rate is rapid, and as a result, charge transfer or activation polarisation is usually small.

(b) Concentration polarisation: or diffusion polarisation appears when the electrode reaction is hindered by mass transport effects, i.e., when the feeding velocity of the reactant and or the removing velocity of the reaction product from the electrode is slower than that corresponding to the discharge current. The diffusion polarisation is dependent on the mass transport properties of the system. Mass transport is a function of temperature, pressure, concentration, and physical properties of the system. In SOFCs, the reactants must diffuse through the porous anode and cathode so the electrode structure is important. Since the electrode reaction rate is a function of the concentration of the reactant gases, the diffusion polarisation becomes more severe as the degree of conversion increases.

(b) Ohmic polarisation. The ohmic polarisation is caused by resistance to conduction of ions (through the electrolyte) and electrons (through the electrodes and current collectors), and by contact resistance between cell components. So cell components and their geometry (thickness) plays a great role in reducing ohmic polarisation. The effect of one type of polarisation is more significant that others at different operating conditions. The figure below illustrates the regions in which various types of voltage losses predominate. From Fig.2-6, it can be seen that at low current densities, the major contribution to the cell voltage losses is from activation polarisation, as indicated by a sharp drop in the cell voltage with increasing current. As the current increases, the resistance polarisation or ohmic loss dominates, as exhibited by the linearity in Fig.2-6 [96]. At high current densities, the cell resistance is controlled by mass transport limitations, resulting in a rapid decrease in cell voltage.

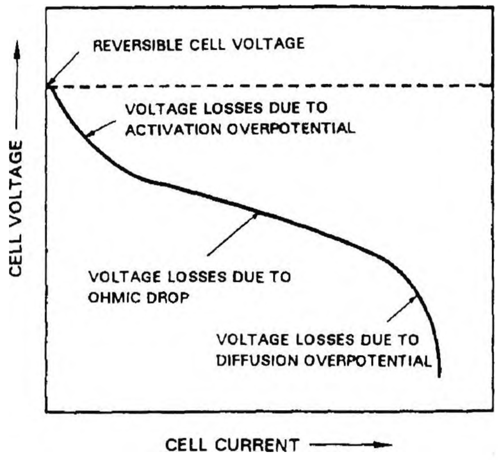


Fig. 2-6 Typical voltage current relation for an operating cell

Conversion efficiency

All practical fuel cells intended for multi-kilowatt or multi-megawatt power generation use hydrogen as a fuel, even if the feedstock is a carbon compound (e.g., a hydrocarbon, alcohol, or coal). The latter must be converted to hydrogen and carbon dioxide via an endothermic reaction with steam followed as necessary by water-gas shifting. In a real fuel cell the objective is to convert as much as possible of the hydrogen in the anode feedstock to work, in order to obtain the maximum overall conversion efficiency. The same will be true for the cathode oxidant stream, unless it is atmospheric oxygen in the form of air. Even if air is used, some net oxygen conversion will take place, since the practical circulation of large amounts of air requires pumping work, which results in an energy loss. Thus, unless process air-cooling is used conversion will be kept at the maximum with good electrochemical performance [97].

In typical systems, conversion of reactants to products occurs as the reactants move across the face of the cell, resulting in a higher current density on the inlet side and a lower current density on the outlet side. Since the cell must have high electronic current-collector conductivity, the electrodes are equipotential surfaces. The maximum theoretical potential the cell can have will be the lowest Nernest potential of the cell. In systems with co-flow of reactants, this will occur at anode exit. While the situation in systems with counter-flow, cross-flow or more complex geometry is not so obvious, in general the cathode reactant utilisation with atmospheric oxygen is usually rather small, so that the anode outlet Nernest potential is a good approximation to the maximum possible cell potential. Since the difference between the inlet and exit Nernest potentials is strongly temperature-dependent due to the presence of the RT/F term, and since $-\Delta G$ falls with temperature, the overall cell performance will be a strong function of the operating temperature of the cell.

2.9- FUEL CELL APPLICATIONS

In recent years, concerns have become more pronounced about the need to balance economic and social changes with long term sustainability and protection of the environment. This is clearly the case in the transportation industry, where the use of combustion engines and fossil fuels has been linked with a number of air pollutants including carbon-dioxide, nitrogen oxide, carbon monoxide, hydrocarbons and particulates. Scientific research has tended to indicate that these pollutants, in turn, have a negative impact on the health of humans and the environment, including respiratory problems, damage to vegetation and aquatic organisms, and global warming.

Consequently, there is growing need for alternative fuel and transportation technologies. Governments have demonstrated a commitment towards the promotion of alternative modes of transportation that improve energy efficiency and air quality. Specifically, a number of initiatives dealing with environmentally sensitive vehicles and fuels are being evaluated, including the use of fuel cells.

In determining whether or not market exists for fuel cell technologies, it is important to consider both the type of product being manufactured and the competitive structure of the industry. The electrochemical fuel cell is a highly efficient technology, which can be used as a power source for buses, stationary power plants, ships and submarines, and automobiles. Specifically, a fuel cell is capable of converting hydrogen into electric power with virtually no detrimental impact on the environment. Consequently, it combines key benefits associated with electric vehicles with fast refuelling capability and a longer range.

Costs associated with degradation in environmental and human health, based upon the production and use of oil and refined fuels in the US, have been estimated at between $11 - $187 billion per year [86]. Recently, government representatives from around the world confirmed (i.e., the 1992 United Nations conference on environment and development) the need for national policies to limit carbon dioxide and green house gas emissions.

A number of constraints must be overcome prior to the commercialisation of fuel cells. First, current hydrogen storage methods are bulky; fuel containers are heavy (accounting for approximately 93 - 97% of the total weight of the fuel storage system) and /or large (e.g., liquid hydrogen systems may not be significantly heavier than gasoline storage systems, but they tend to be significantly larger). While this might be less of an issue with transit vehicles, it remains a significant limitation in terms of smaller passenger vehicles. Second, there are also concerns about the need for a new fuelling network. In light of the prototype status of fuel cell transportation initiatives, there remains a need to develop hydrogen storage, delivery and production systems to support wider use. However significant advances have been made in this area, including photovaltaic technologies and research into alternative fuel bases such as ammonia, methane and biomass.

Solid oxide fuel cells are mainly suitable for stationary power plants due to the high operating temperature. Applications range from mega watt plants to small plants for buildings. The United States, Japan, and Europe are all actively developing SOFC for commercial applications. The U.S. Department of Energy (DOE) is sponsoring a considerable amount of research and development activity to develop SOFCs at various corporations and other organisations, as are the Electric Power Research Institute (EPRI) and the Gas Research Institute (GRI) [86].

Westinghouse [132] has been involved in SOFC development in order to commercialise tubular SOFCs for nearly three decades. Presently, DOE and GRI are supporting tubular SOFC technology development at Westinghouse. Several 3-kW tubular SOFC power units have been constructed and tested for extended periods of time.

The high operating temperature and tolerance to impure fuel streams make the SOFC system ideal for utilising H_2 and CO from natural gas stream reforming and coal gasification plants, in which its high quality waste can be used either in bottoming cycles and/or to provide all or part of the process heat gasification.

Future application of the system must be seen in the context of the economics versus its potential competition, namely gas turbine combined cycle systems and systems using other fuel cells. A major technical challenge in SOFC technology is the fabrication of the component layers of the electrochemical cell stack and reducing the cost of fabrication. This will eventually prove a break through towards commercialisation.

2-10 MARKET INTRODUCTION OF SOFCs

In the view of the customer, a fuel cell must appear exactly like a conventional CHP, as a compact plant, which will be supplied with natural gas and delivers electricity and heat. Furthermore, the customer naturally demands a high level of efficiency and a low level of exhaust fumes and noise emissions, high levels of availability, low capital requirement, and low maintenance costs. The demands with regard to efficiency and emissions are best fulfilled by the fuel cells due to their specific properties. Proof of the availability and maintenance costs must be produced through practical testing of the SOFC, which is still in its initial stages. The considerable challenge facing the developers in the medium-term in the reduction of the production costs, so that the fuel cell as CHP comes into direct competition with conventional technology (e.g. gas engines and gas turbine CHPs). The specific investment costs presently stand at $1000 – 2000 per kilowatt depending on plant size and plant specifications demanded [43]. With that, the target costs for the SOFC have been set.

Today we find ourselves at the stage where the SOFC-technology is, firstly, being tested for demonstration at a larger scale. It is yet to be proven that the high expectation of the public for such technology can be fulfilled. Here, the tubular concept currently has a clear advantage over the planar concept.

The market for fuel cells will go up mainly in regions with sufficient natural gas supply and natural gas distribution networks, for which it will be assumed that the importance of natural gas will increase world-wide in the next few years. In the medium-term, Europe, North America and Japan in particular, can be named as the main focus.

The target for the planar concept at Siemens is to put the first 100 kW-plant in operation in 2002/2003 [18]. The development and commercial market introduction of bigger pressurised operating systems in the 1 MW-region should be successfully concluded by 2010.

Assuming that the technical problems still existing today are solved, reduction of the present high cost to competitive levels through simpler and new production methods remains a substantial task for the developer. Initially, the purchasing decision of the customers is influenced by the investment cost, and ultimately by the life cycle costs as well. Only at a competitive price and additional nonmonetary advantages, like the environment, for example, can a market-share be acquired. To this end, design methodologies than target cost reduction, improved quality and understanding of the product need to be adopted.

CHAPTER-3

Design methodology- literature review

3.1- Introduction

Designing is not something that has always been regarded as needing special abilities. In traditional, craft-based societies, there is usually no prior activity of drawing or modelling before the activity of making the product. For example, a potter will make a pot by working directly with the clay, and without first making any sketches or drawings of the pot. In modern societies, the design activity usually commences with some form of design intent, outlining a need to be met, and which can be represented as design briefs or objectives, including customers' requirements (which may be vague). The recent past has witnessed a growing interest towards the adoption of new methodologies to design. A design methodology can be defined as any identifiable way of working, within the context of designing. There has been a substantial growth of new unconventional procedures that are more usually grouped together under the name of 'design methods'. The main intention of these methods is that they attempt to bring rational procedures into the design process. These methods have been used by the Japanese over the years, but were not adopted by the western world until recently.

3.2- PRODUCT DESIGN & SPECIFICATION

In determining a product specification, conflict and misunderstanding can sometimes arise between the marketing and the engineering members of the design team. These are usually because they focus on different interpretations of what should be specified. Managers and market researchers tend to concentrate more on specifying the desirable attributes of a new product (usually from customers' point of view) where as designers and engineers concentrate more on product's engineering characteristics (usually in terms of its physical properties).

If properly understood, confusion can easily be avoided. Designers make decisions about the products physical properties, and thus determine engineering characteristics; but those characteristics then determine the products attributes, which in turn satisfy the customer's needs and requirements.

It is necessary to understand just what customers want in terms of product attributes and to insure that these are carefully translated into specifications of the appropriate engineering characteristics. This attitude towards product design is based on the philosophy of 'listening to the voice of the customer', and is reflected in an increased concentration on product quality. Design for quality is recognised as a major factor in determining the commercial success of a product [34].

A comprehensive method for matching customer requirements to engineering characteristics is the quality function deployment method. The method recognises that the person who buys (or who most influences the buying decision for) a product is the most important person in determining the commercial success of a product.

Cross [34] stated that if customer do not buy it, then the product however 'well-designed' would be a commercial failure.

3.3- QUALITY FUNCTION DEPLOYMENT (QFD)

This is a formal method primarily designed to accommodate the customer requirements into the design and manufacture of products. It is an important tool to facilitate multi-functional planning and communication in a concurrent engineering product development environment. It provides a structural framework to translate the ‘ voice of customer ‘ into the actions needed to meet customer expectation. QFD moves from customer requirements, through design requirements, part characteristics, and process planning, to the detailed operation requirements. Therefore, if QFD is implemented properly, customer requirements can influence the functional areas of the company that are often isolated from adequately knowing and reacting to the needs of their customers. Dr. Shigeru Mizano of the Tokyo institute of technology originated the QFD methodology in the late 1960s and early 1970s in Japan [6]. In 1972, Dr. Mizano used quality tables to help support planning, and these later evolved into QFD. Hauser and Clausing [68] state that QFD originated in 1972 at Mistibushi’s Kobe shipyard site. Toyota autobody began using QFD in 1977 and has experienced significant benefits, including a 40% reduction in the development cost for a new model and 50% reduction in development time [3]. QFD has been used successfully by Japanese manufacturers of consumer electronics, home appliances, clothing, integrated circuits, synthetic rubber, construction equipment, and aircraft engines. QFD was introduced into USA in 1983, essentially through the Ford Motor Company. Since then, the application of QFD in the United States has been growing at a significant rate [119].

At the Ford Motor Company in the 1989 alone, there were 80 to 90 QFD studies underway, and most of the 2600 engineers in the body and chassis group had taken training in QFD. Boeing, Hughes, Digital Equipment, Hewlett-Packard, AT&T, and ITT are also reported to be using QFD for a variety of products [119].

QFD is a cross-disciplinary activity that can involve all pertinent organisational functions of a company, and is usually implemented by a mixed-discipline design team, consisting of members from marketing, design, manufacturing, logistics, maintenance and finance. The major work of conducting QFD is centred around filling a number of translations to process from the customer requirements to the detailed control of operations. The number of translation matrices is determined by the properties and complexity of the product, as well as by the level of detail required. However, the structure of all translation matrices is similar. The first translation matrix, which is often called the 'house of quality', has the most general structure. It shows the relationship between the customer requirements and the specific design or engineering requirements. Additional information is also given on the correlation between the engineering requirements, the degree of competitiveness, and on technical and cost assessments of the design or engineering requirements.
The method starts with the identification of the customers and of their requirements and desired product attributes. There are various market research techniques that can be used to assist the gathering of information about customer requirements and preferences. Usually, of course, customers will talk about products in terms of both general attributes and specific characteristic observations. Some are trivial while others are imperative. As in the performance specification method, it may be necessary to interpret their observations into the designer's perceptions of what the customers really want. For this reason, all the detailed customer requirements are retained in statements of product attributes, even though they may be imprecise.

QFD has three major objectives (to identify who the customer is, what the customer wants and how to fulfil the customer's wants). The Japanese give a strong importance to the word deployment. Deployment in Japan means extending involvement or broadening of various activities. QFD in Japan is considered as the best tool which spreads awareness on the need to focus on customer requirements and encourages company-wide responsibility and commitment towards achieving quality standards which would be consistent with customer expectations and the companies' own aspirations.

At this stage, it is important to define QFD, show how it works, present some of its benefits, and explain its relationship with other continuous improvement programmes such as total quality management (TQM), statistical process control (SPC), and concurrent engineering (CE).

The power of QFD is in its effectiveness in re-examining customer defined *hows* in order to establish the true customer *whats* [112]. There are many attempts to define QFD that have been widely reported in literature.

Lynch and Cross [90] define QFD as a system for designing a product or a service based on customer wants, involving all members of the supply organisation. As such, it is a conceptual map for inter-factional planning and communication.

Hauser and Clausing [68] view QFD as a set of planning and communication routines. "QFD focuses and co-ordinates skills within an organisation". First to design, then to manufacture and market goods that customers want to purchase and continue to purchase. The foundation of the QFD is the belief that products should be designed to reflect customers' desires and tests- so marketing people, design engineers, manufacturing staff must work closely together from the time a product is conceived.

Garvin [57] states that QFD may be defined as elaborate charts to translate perceptions of quality into product characteristics and product characteristics into fabrication and assembly requirements. In this way "the voice of the customer" is deployed through out the company.

Whether QFD is viewed as a process, a method, a system, or even philosophy, it ensures that customer requirements are integrated into new products as early as the design stage. It is a systematic means of ensuring that customer or market place demands are accurately translated into relevant technical requirements and action through each stage of product development [53,92]. It is therefore necessary to survey customers and discuss these needs. In many of the Japanese companies, which implemented QFD, customers are brought in and participate in the design of the product with teams of design and manufacturing engineers.

Quality function deployment can lead to a wide variety of benefits [140], it can help:

- define product specifications meeting the customer's requirements, while paying attention to the competitors;
- ensure consistency between the customer's requirements, and the measurable characteristics of the product;
- inform and convince all those responsible for various stages of the process of the relationship between the quality of the output of each phase and the quality of the finished product;
- ensure consistency between the planning and the production process;
- Get things moving more quickly because planning takes place at an earlier stage and mistaken interpretations of priorities and objectives are minimised.

Adao [63] conducted a survey on QFD spread in Japanese industry. The survey concluded that the following benefits were reported by companies using QFD in their business processes. QFD enables organisations to achieve the following:

- Translate customer requirements into meaningful (technical) requirements at each stage of the development and production processes.
- Brings people together from various disciplines and facilitates the formation of teams capable of meeting customer requirements.
- Squeezes the design time up to 50%.
- Increases customer satisfaction and reductions in warranty claims.

There is a strong relationship between QFD and many of the continuous improvement programmes such as statistical process control (SPC), concurrent engineering (CE) and total quality management (TQM). The Japanese who have pioneered QFD strongly believe that QFD can only be effective if it is strongly linked to a wide and encompassing quality programme. This is because QFD starts with the objective and works backward by establishing the customer-supplier chain, which is capable of delivering to the end customer. It really maps the whole innovation process and ensures that there is a wide involvement and corporate ownership of innovating activity. Kogure and Akao [82], stated that QFD activities should not be confined to the process flow between upstream and downstream, but must be systematised to involve different levels of management, such as top executives, managers and engineering staff. Used in that way, it can help management apply company-wide quality control as a truly effective corporate strategy.

QFD is more concerned with design aspects and tends to work backward by starting with the end objective and then determining means by which the objective is achieved. SPC on the other hand is more downstream and is concerned with process improvement, the prevention of defects and the reduction of variability. QFD does not seek to replace SPC and the two techniques are very much compatible with each other. In addition to the prevention of product defects and process variability, both downstream activities, QFD makes ‘right first time’ and ‘zero defects’ both tangible goals since it aims at optimising design for manufacturability and reflecting true customer requirements.

Concurrent engineering (CE) also referred as design for manufacturability or parallel engineering is one other improvement programme that is strongly linked with QFD. CE attempts to optimise the design of the product and manufacturing process to achieve reduced lead times and improved quality and cost by the integration of design and manufacturing activities and by maximising parallelism in work practices [24].

QFD is a great opportunity for making concurrent engineering work. Its main principle is bringing people together representing different functions to agree on key parameters of the product, process and manufacturing methods. CE is a concept which was difficult to apply in the past because it tended to be initiated by certain groups of people without widening the involvement and without any serious attempt to change the culture of "business as usual". Basically, QFD helps establish the customer-supplier chain by getting rid of *over the wall engineering*.

Concurrent engineering takes over from QFD to ensure that the voice of the customer is used for the design of the production process. Its purpose is to improve the quality of process design and also to increase design efficiency.
The management of core processes based on QFD and simultaneous engineering practices is the best way of delivering innovation of high quality, at the right time, to the right customer and in the right quantities in a consistent manner. Managing core processes in this format is also the best way to investigate the "never ending improvement" philosophy as the above practices are constantly subjected to review and updating.

There are however various problems with the use of QFD. The following problems are identified to be associated with its implementation [112]:

- Engineers think that QFD is a false science, too focused on the mechanics of scoring.
- It takes a long time to develop a QFD chart fully.
- Team members get caught in the details of the exercise while the market window closes on them.
- Getting into too much detail (QFD tables become unmanageably large).

3.3.1- CUSTOMER INPUT IN THE HOUSE OF QUALITY (HOQ)

QFD is based on customer input, also called ‘the voice of customer’. The process from the collection to the final rating of customer input consists of the first four steps of HOQ.

Customer needs(whats) the first part of customer input is to determine what are the needs of customers for the product concerned. Customer needs are usually expressed in customers’ words that can be collected by focus groups or individual interviews. According to Griffin and Hauser [61], individual face-to-face interviews may be more cost effective than focus groups, and 20-30 customers should be interviewed to obtain 90-95% of all the possible customer needs. Mail/telephone surveys are not suitable for collecting qualitative data such as customer needs due to the difficulties in controlling the scope of responses.

Customers’ words are usually too general and/or too detailed to be directly used as customer needs. To facilitate analysis and application, the words collected are usually organised as a tree-like hierarchical structure to form various levels of customer needs and, according to the situation, those at a specific level are chosen as the final customer needs. An Affinity Diagram, a method of arranging random data into natural and logical groups, can be used for this purpose [22,33].

Relative importance rating the second part of customer input is to rate the importance of the customer needs. The company would work on the most important customer needs and disregard the unimportant ones to make best use of its resources. Conveniently, customers are asked to give relative importance ratings for each *what* using 5-, 7- or 9-point scales. More elaborate scales, such as the 1-to-10 scale and anchored scale, are also used [61]. A common and appropriate way of obtaining this information is mail/telephone surveys. Since sufficient number of customers should be surveyed to provide statistical significance, focus groups and individual interviews are usually not suitable for collecting quantitative information about the relative importance of customer needs due to their high costs.

Competitive analysis The third part of customer input is to rate the product performance of the company and its main competitors, so that the competitive positions of the company's product in terms of the customer needs can be assessed. Knowing the company's strengths and weaknesses in key aspects of a product relative to its main competitors is essential for achieving competitive advantages. Asking the customers to rate the relative performance of the company's product and its competitors' products of a similar type on each *what* using specific scales can do this. As in step 2, a useful way to obtain this kind of information remains mail/telephone surveys, and focus groups and individual interviews are still not suitable here. It should also be noticed that customers can and should only rate the products they use and are familiar with. Thus, many more customers should be sampled to retain statistical significance. Another set of ratings of the customer needs, called competitive priority ratings for the company, can be obtained by analysing the company's relative positions from these customer perceptions, usually using the sales point concept [22,33,118].

For each *what*, combining the relative importance perceived by customers in step 2 and the company's competitive priority in step3, final importance ratings of the *Whats* can be obtained for the company's product. *Whats* with high final ratings indicate high potential business benefit to the company.

3.3.2- QUANTITATIVE PRESENTATION OF QUALITATIVE REQUIREMENTS

Typically, customer expectations tend to be vague items, such as " I want high reliability". The requirements need to be more measurable. However, this step can be one of the most challenging efforts in the QFD process. Each product measure should have the following characteristics.

- It should be measurable; you should be able to define its units of measure and method of measurement.
- It should be assigned a target value that, when met, will assure customer satisfaction. These target values should be realistic.
- It should not be design specific; it should not force developers to use certain parts in the design. This characteristic allows for innovation in design.

For practical implementation, the above-summarised steps for collecting and analysing the customer input need to be quantified. Chan [29] proposed a four-step technique to convert the customer requirements in words into quantitative values.

Step 1. There are m customer needs (*Whats*) for the product which are structured and identified from the customers' words, denoted as $W_1, \ldots\ldots W_m$.

Step 2. There are q customers surveyed. Each is asked to provide relative importance ratings for the set of m needs. Averaging these q sets of ratings, the relative importance ratings of the customer needs, $g=(g_1, \ldots . g_m)$, can be obtained. For g to be representative of the population of potential customers and for the surveys of k competing companies to be statistically significant, q should be sufficiently large.

Step 3. There are $(k-1)$ competitors identified which manufacture products of a similar type, denoted as $C_2, \ldots, C_k$. The company under study is denoted as C_1. The same q customers are asked to rate the performance of the products they use or are quite familiar with for the m needs. Suppose that q_i customers rate the performance of C_i's product. Averaging these q_i sets of ratings, C_i's performance on the m customer needs can be obtained as $x_i=(x_{1i}, \ldots, x_{mi})$. Thus, we can have the following performance rating matrix of the k companies on the m customer needs:

$$X = \begin{array}{c} w_1 \\ w_2 \\ w_m \end{array} \begin{bmatrix} x_{11} & x_{12} & x_{1k} \\ x_{21} & x_{22} & x_{2k} \\ x_{m1} & x_{m2} & x_{mk} \end{bmatrix}$$

Based on this X information, competitive priority ratings of the customer needs can be obtained.

Chan [29] proposed to use triangular fuzzy numbers to represent the assessment of customer needs $w_1, \ldots, w_m$ in step 2 above. In traditional approaches, customers are asked to assign positive numbers to the *w*'s with a small number indicating unimportance and a large number importance. In marketing and psychological practices, there are many scales to measure and quantify qualitative attributes. As people's assessment of an attribute's importance is usually expressed in linguistic terms such as

'unimportant' and 'very important' and then transferred to crisp numbers, a frequently used scale is the 9-point scale:

very   very
unimportant   unimportant   medium   important   important
1-----------2----------3----------4----------5---------6---------7----------8------------9

The rationale of such a 1-to-9 rating scale is justified by the many tests made by Saaty [110]. It is simple and easy to use and also includes enough information that people provide on the attributes measured. However, it is also well recognised that people's assessments of qualitative attributes are always subjective and thus imprecise, and the linguistic terms that people use are to express their feeling or judgements are vague in nature. Using objective, definite and precise numbers to represent linguistic assessments are, although widely adopted, not very reasonable. Chan [29] states a more rational approach is to assign an interval to a vague linguistic term so that its vagueness can be captured. For example, instead of using numbers 7 and 9 to represent important and 'very important' respectively, we may assign intervals {6,8} and {8,10} to these two linguistic assessment terms to express their vagueness. In mathematics, this idea can be built into the framework of fuzzy set theory and triangular fuzzy numbers (TFN) can be used to represent people's subjective assessment. TFN is a special fuzzy set represented by an interval, whose arithmetic is quite intuitive and similar to that for crisp numbers.

Fuzzy set theory Fuzzy set theory, first introduced by Zadeh [139], was developed for solving problems in which descriptions of activities, observations and judgements are subjective, vague and imprecise. The term fuzzy generally refers to the situation in which no boundary for the activity or judgement can be well defined. This notion of fuzziness is common in our everyday life, such as the class of 'important' customer needs, the class of 'nice' cars, etc. These classes of objects cannot be suitably described by traditional set theory in which an object is either in a set or not and cannot partially belong to a set, but they can be well represented using fuzzy set theory.

A triangular fuzzy number, denoted as M=(a,b,c), where a ≤ b ≤ c, is a special fuzzy number, which, representing a fuzzy set or concept M = 'approximately b', has the following triangular-type membership function [74]:

$$U_m(x)\begin{cases} 0 & x \le a...or..x \ge c \\ (x-a)/(b-a) & ....a \le x \le b \\ (c-x)/(c-b).... & b \le x \le c \end{cases}$$

Within the framework of the fuzzy set theory, instead of assigning definite ratings of 1 to 9 to represent the assessments of customer needs form 'very unimportant' to 'very important', we express them as special fuzzy sets from M1 approximately 1 to M9 = approximately 9 in order to take the impression of people's qualitative assessments into consideration. These fuzzy sets are specified as suitable triangular fuzzy numbers shown in the scale below.

very unimportant   unimportant   medium   important   very important

M1--------M2--------M3---------M4-------M5------M6-------M7--------M8---------M9

[1,1,2] [1,2,3] [2,3,4] [3,4,5] [4,5,6] [5,6,7] [6,7,8] [7,8,9] [8,9,9]

Benefits of the QFD process

- QFD requires a cross-functional team from marketing, design, and manufacturing. Having a team accountable for realising a product from concept to manufacture improves communication across functional groups and reduces the chances that the design team will design a product that is unmarketable or unmanufacturable.
- The complete QFD process integrates the information that each specialised group in an organisation provides to the next group in the development process, assuring that customer requirements are translated into a manufacturable, marketable product.
- QFD assures that the team constantly focuses on items that will most influence achieving customer satisfaction. Only the key items in each phase are carried onto the next phase.
- QFD provides the team with the appropriate information for making decisions in the product realisation process. This information includes customer priorities, influence of measure on customer satisfaction, and technical difficulty ratings.
- QFD provides a structured methodology for managing performance requirements, which, in turn, aids project management.
- QFD also comes with a standard documentation format. This format provides the team with easy traceablity of the deployment of customer requirements to manufacturing operations.

3.3.3- QFD LIMITATIONS

QFD has paid less attention to the quantitative design and optimisation. It focuses more on the customer requirements and quality improvement with out integrating a mathematical approach into the design process.

The emphasis of the current QFD applications to maximise product quality is also technically one-sided in a sense that it assumes infinite resource availability to meet the targets and thus ignores any economic constraints. It neglects the fact that a manufacturing company is usually an economic enterprise, which is under constant pressure to trade-off between quality and cost. However, product design is not simply a maximising effort but an optimising process as well.

In practical applications of QFD, engineering tasks are not prioritised according to their quality contributions per unit cost incurred. Technically one-sided design only considers what quality level can be achieved through meeting respective engineering targets, where as an economic design can tell what quality improvement can be gained per unit financial investment. Economic prioritisation can ensure that maximum customer satisfaction is achieved under the resource constraints. To account for the cost of a quality, Bode and Fung [19] developed a model for the trade-off between product cost and product quality as a linear program. The model attempts to maximise total customer satisfaction as a function of the resource allocated and quality improved. The optimum solution of the linear program is obtained by allocating the budget to the attainment of technical attribute targets in a descending sequence of their ratios. Thus, customer satisfaction can be maximised by committing resources to technical attributes with which one cost unit can buy the highest return in customer satisfaction.

3.4- DESIGN FUNCTION DEPLOYMENT (DFD)

Design function deployment (DFD) has been developed as a comprehensive design system incorporating the advantages offered by quality function deployment (QFD) concurrent engineering and design models, methods and systems [116].

Design function deployment is an alternative approach to QFD to create a product design strategy, which embraces the concurrent engineering environment and all customer requirements within a free flowing information structure. It is a design system, which incorporates the features of prescriptive design model and design methods for the integration of manufacturing. This system enables the building of quality into the design by developing a quality plan derived from customer requirements [73]. DFD starts with the identification of the need for a product or process from customer's point of view. All relevant data is recorded to insure consideration of all specifications in the design process as well as for future reference. The recorded customer requirements are then translated into design requirements that include specifications and constraints. The word customer not only refers to the people who will use the end product but also the people who are involved in the design process such as the assembly department, component manufacturing department and the company responsible for financing the project [73]. There can be several requirements made by customers on a product, some of, which are imperative while others are desirable. A relative weighting system should therefore be employed to classify customer requirements. Importance rating comes from customer requirements weighting, market relative importance and the designer's technical design functions all optimised to give a maximum advantage. DFD insures all relevant requirements and specifications are given consideration. It focuses in getting the design right the first time round. It also facilitates design retrieval that enables the use of an experience gained during the process of design in the past [73]. Traditional ways of design systems lack this facility and prevent these advantages from being taken. DFD maximises knowledge about performance at the design stage. In traditional methods, critical design decisions are made before an adequate knowledge on performance. Concurrent engineering helps delay design decisions and closes the gap between decision making and knowledge of performance. Engineering change notices are a major cost driver and there can be considerable difficulty in apportioning costs, especially if subcontractors are involved. Use of DFD charts makes it easier to assess the implications of changes and identify which decisions need to be revised. The output of the DFD process is a design which has been validated against all the constraints and optimised for some, or many, parameters. Quality is an obvious parameter to optimise for, but it implies a definition and a method of measuring quality.

DFD defines the quality as " The marriage between customer importance rating, which comes from customer requirements weighting, the bench mark position desired by the designer in the market, market relative importance (sales advantage) and the designer's technical design function, prioritised to give maximum advantage" [11]. The formal DFD design process is a focussing exercise which highlights the customer's requirements and gives these priority. There are several different customers, both internal and external, and by regarding the designer as a customer all the appropriate constraints can be considered simultaneously, giving a concurrent design methodology.

DFD charts are similar to QFD 'house of quality' charts, but DFD contains several additions and extra capabilities. QFD tends to be a reactive system, documenting what already exists. DFD is proactive system, good for original design as well as modifications, which considers all possible options [11]. The definition of customer has been expanded in DFD to include everyone who requires something out of the design process, not just the organisation paying the bill. There are also a number of design tools included in the overarching DFD design methodology. Robust Engineering helps design out dependency on close tolerances, which can be applied to variations in the manufacturing process as well as component dimensions. Taguchi techniques can be used to determine relative importance of parameters and decrease dependency on some of them. Failure modes and effects analysis increases reliability [74].

Design retrieval and concurrent engineering is inherent in the DFD method. Trade off and conflict analysis is easily implemented and techniques for design optimisation are available. An important step in the DFD process is to record the design issues in a solution neutral form before considering possible alternative solutions [50]. The charting process records how the design evolved, and why one option was chosen and not others.

3.4.1- DFD MODEL

The design model for design function deployment has five stages.

1- *Translating customer requirements into design specifications.*

Design problems are always set within limits. One of the most important limits is that of cost. What the client is prepared to spend on new product or what customers are expected to pay for a new product. Other common limits include performance, acceptable size or weight of the product etc. Customer requirements are carefully analysed and translated to design functions, which set limits to what has to be achieved by the design thereby limiting the range of acceptable solutions. Care must, however, be taken in translating customer requirements as it sets up boundaries to the solution space within which the designer must search. Not all the identified requirements will be equally important to customers. The design team will want to know which attributes of their product design are ones that most heavily affect customers' perception of product, and so it is necessary to establish the relative importance of those attributes to the customers themselves. A list of customers' requirements in their own words are established. After recording the requirements, manufacturing constraints, environmental requirements, company requirements and statutory requirements are added to the list. These rated requirements are then deployed as design requirements in a solution neutral form, which are called step-1 design functions.

2- Conceptual solution

After a thorough consideration of the requirements and constraints and translation to design functions, possible conceptual solutions are established. Here, several different design concepts are proposed to meet the design specifications. Some of these solutions may not be cost effective, efficient or even realisable. A careful analysis and evaluation is made and promising solutions are taken to the next stage. The solutions that are not taken to the next stage due to some constraints are stored for future use. This is how DFD comes useful for design retrieval and future modification and redesigning. Generation of conceptual design involves taking the statement of the problem and generating broad solutions to it in the form of schemes. It is the phase that makes the greatest demands on the designer, and where there is most scope for striking improvements. It is the phase where engineering science, practical knowledge, production methods, and commercial aspects need to be brought together and where the most important decisions are made. Within Design Function Deployment, the statement of the problem is established at the end of the analysis on customer requirements.

The main kernel of the design activity is the generation of conceptual solutions, whether it is at a higher level when considering the overall system architecture or at a lower level when deriving parts of an architecture or layout. Within the various engineering disciplines, several methods or techniques have been used in the generation of conceptual solutions. Such methods include:

Morphological analysis: which derives its name from the dictionary definition: pertaining to the study of organised system or form, can be considered to be a systematic approach to discovery and invention. It is used to force divergent thinking and to safeguard against overlooking novel solutions to a design problem [75].

Exploration of existing concepts: This involves the exhaustive exploration of existing and proven design concepts which have been used to satisfy similar requirements or needs, by looking at various sources of information. Such information sources include: books, research papers, design concept catalogues as well as studying actual products and systems.
Analogies: This is considered as an effective method of generating solutions and it involves a wider and less obvious range of design solutions from various analogous sources. An important source of analogies is living organisms [52].

Brainstorming: This is an approach used to stimulate a group of people to generate many new ideas as quickly as possible. It provides conditions in which a group of open-minded people from as many different fields or disciplines as possible.

3- Detailed design stage

Each of the conceptual solutions are taken individually and divided into sub systems. Alternative solutions for each sub system are proposed. At this stage one comes up with working drawings and parts list. There may still be different layouts. The design at this stage is still an abstract, as materials for various parts have not yet been selected.

4- Manufacturing and materials selection stage

Manufacturing process is directly affected by the choice of material for the parts. Each part in each layout is considered. Taking into account the part requirements and constituting material, a rough idea about its geometry can be established. Different manufacturing techniques are then analysed and an optimum one selected. Cost and manufacturability are the dominant factors at this stage.

5- Planning stage

This is the final stage of the design process before mass production commences. Here, all the process characteristics that were established earlier are recorded for the layout. Master production schedule for each part is established. This includes information about operation planning, quality economics and quality control details.

3.4.2- DFD CHARTS

Several groups of information are generated at each of the first four stages of design function deployment. These are stored in a QFD style chart which is called the main DFD chart. It has seven sections of groups of information. Each group has five stages on the design process [73].

(1) The whats

The *whats* are the requirements set by customers in their own words. These include the end product user's explicit requirements, manufacturing constraints, maintenance and user environment, company requirements and legal requirements. The requirements may be very broad, that require refinement.

After the customer requirements are carefully recorded, they are classified into primary, secondary and tertiary (Fig.3-1). The primary customer requirements are the broad requirements, which are basic to the product and represent strategic customer requirements. The secondary requirements are somewhat detailed in nature and are refinements of the primary requirements and can be considered as tactical customer requirements. Thus, a primary customer requirement may constitute more than one secondary requirements. Each of the secondary requirements can be further refined into specific requirements, which are called the tertiary requirements. This classification allows the customer requirements to be equal in status and information content, and similar in generality, so that, likes are compared with likes when assigning relative importance ratings to them. Tertiary requirements are then treated as the customer requirements for deployment or translation to design functions. The designer is responsible in rating the tertiary customer requirements by combining the degree of importance to the customer, Sales advantage and any other design considerations.

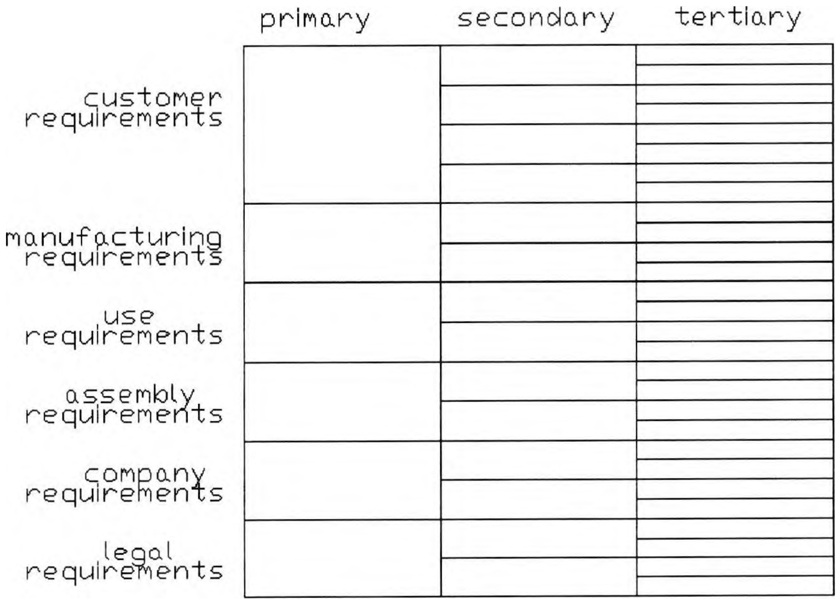


Fig. 3-1 Classified list of customer requirements

(2)- The hows

The designer translates the *whats* into design functions called the *hows*. These functions are the identifiable and actionable design requirements translated from customer and other requirements or design functions which insures the satisfaction of the initiating customer requirements and the quality performance of the resulting product. These functions are established in a solution neutral form at the initial stage. The *hows* are technically precise design specifications as written by the designer. Design functions can also be classified into primary, secondary and tertiary functions. The tertiary customer requirements are considered one by one and checked whether any of the already generated design functions deploy the current customer requirements (Fig.3-2). It might be necessary to add more design functions to fully deploy the requirements at this stage.

HOW WHAT	function-1	function-2	function-3	function-4		
requirement-1		3				
requirement-2	9		1			
requirement-3			9			
requirement-4						

Fig.3-2 Relationship matrix

(3)- The relationship matrix

This matrix has entries at the intersection of the *whats* and the related *hows* as in Fig.3-2. The entries are indicators of the strength of relationships between the customer requirements (*whats)* and design functions (*hows)*. There are two common ways of completing the relationship matrix. A numeric or symbolic representation can be used to represent a weak, medium and strong relationships respectively. This allows easier interpretation of relationships and allows cross-checking of blank rows or columns. These indicate that we either have a redundant design function or functions are not doing anything to satisfy a particular requirement. At a later stage the numbers are given a positive and negative sign indicating if relationships are supportive or conflicting.

4-The interaction matrix

This matrix shows how the design functions interact with each other. There are two aspects associated with interactions. One focuses on the problem, establishing a supporting or conflicting design functions; the other focuses on the solution which involves designing out conflicts. Two similar charts are used separately for the analysis of the interactions between the design functions.

(4a)- Problem related interactions

Now the design functions are considered for interactions with an intention of identifying and resolving conflicts. In the first instance the conflicts are analysed with a problem-focused outlook. This involves exploring interactions between each specification and constraint, and establishing how they all influence each other positively or negatively. This analysis may result in consultations with customers and redefining the customers' requirements. The interaction table attached to the design functions establishes the correlation between the *hows*.

The functions could be in support or conflict with each other. A numeric representation is used to indicate the type of interaction. Commonly used values are:

+2 for strong positive interaction
+1 positive
-1 negative
-2 strong negative.

Positive indicates functions are in support where as negative indicates a trade off is needed as functions are in conflict. A blank indicates that there is no interaction between functions. As shown in Fig.3-3, function 5 is in conflict with two other functions. One can identify at a glance that function 5 needs to be modified or eliminated depending on its effect in the over all product quality. Functional importance, however, needs to be considered. Function 5 might happen to be the most important of all. This is where trade off and/or compromise comes into place. One should, however, look at the design with a view to making the trade off go away before attempting it.

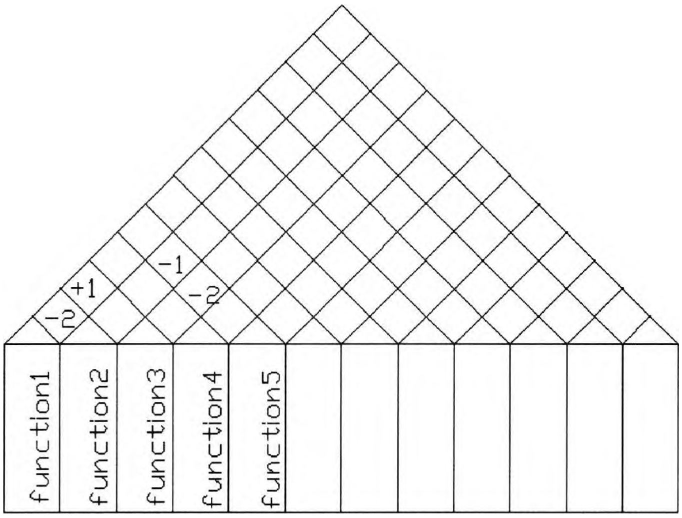


Fig. 3-3 Problem oriented interactions

(4b)- Solution related interactions

Once the problem-focussed analysis is completed a solution-focused analysis is conducted as shown in Fig.3-4, where by the requirements are modified (i.e. eliminated, combined, translated). This provides a guaranteed opportunity to analyse the problem for consistency. Action needs to be taken depending on the level of interactions between the design functions. This will combine analysing the problem-related interactions, considering functional importance and using common knowledge to resolve all the conflicts and/or perform trade-offs between design functions.

The solution based interaction table uses interaction values:

1-eliminate
2-combine
3-transfer
4-modify

This is a course of action as opposed to mere interaction level, which comes at a later stage of the design process. It focuses on the decision that needs to be taken which is useful for subsequent generation of alternative design concepts.

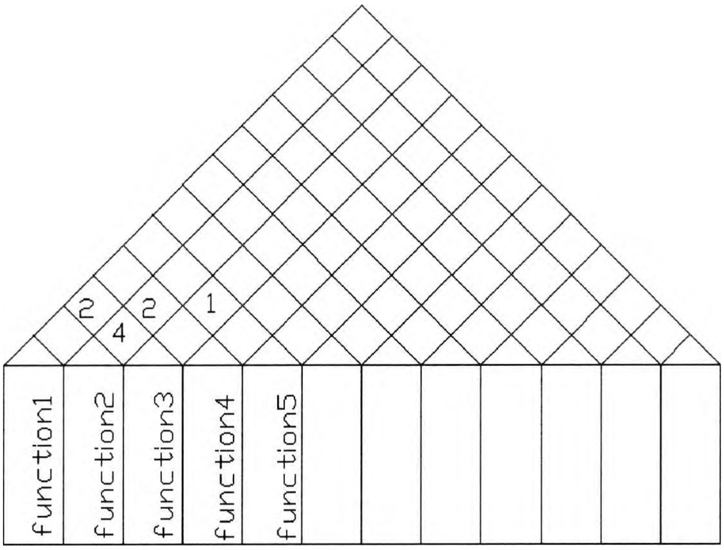


Fig. 3-4 Solution oriented interactions

(5)- Target values

After the design functions are lied out, target values information is established for each function. This is sometimes known as the how much design function. The target values are basically reflections of system performance, maintenance procedures, wear and tear and so on. At the specification level, the target values may not be fixed accurately and experimentation may be necessary to decide on the values. The target information consists of: Upper limit of target value, lower limit, nominal target value, confidence level, and Improvement direction of target value Expressed as:

'+' The higher is the better;

'0' The target is best;

'-' The lower the better.

The target information provides targets for future improvements. It also serves as a yardstick for performance achievement.

(6)- Degree of importance

Some of the customers' requirements can be very important to the customer and may influence heavily his/her decision to purchase the product. There may be some other requirements which may not be so important but are desirable. These varying degrees of importance for each of the tertiary customer requirements are also established by the customers. In this way the customer requirements and their importance ratings are established.

The degree of importance is an important part of the quality plan. Weighting factors are assigned to the *whats* depending how the customers (which include end user, sales department, manufacturing, legal bodies, and the designer) rate the requirements. The ratings can be categorised into relative and absolute ratings. Relative importance is the figure assigned by the customer in a scale of 1 to 9. All the above groups of information are contained in the main DFD chart shown in Fig.3-5.

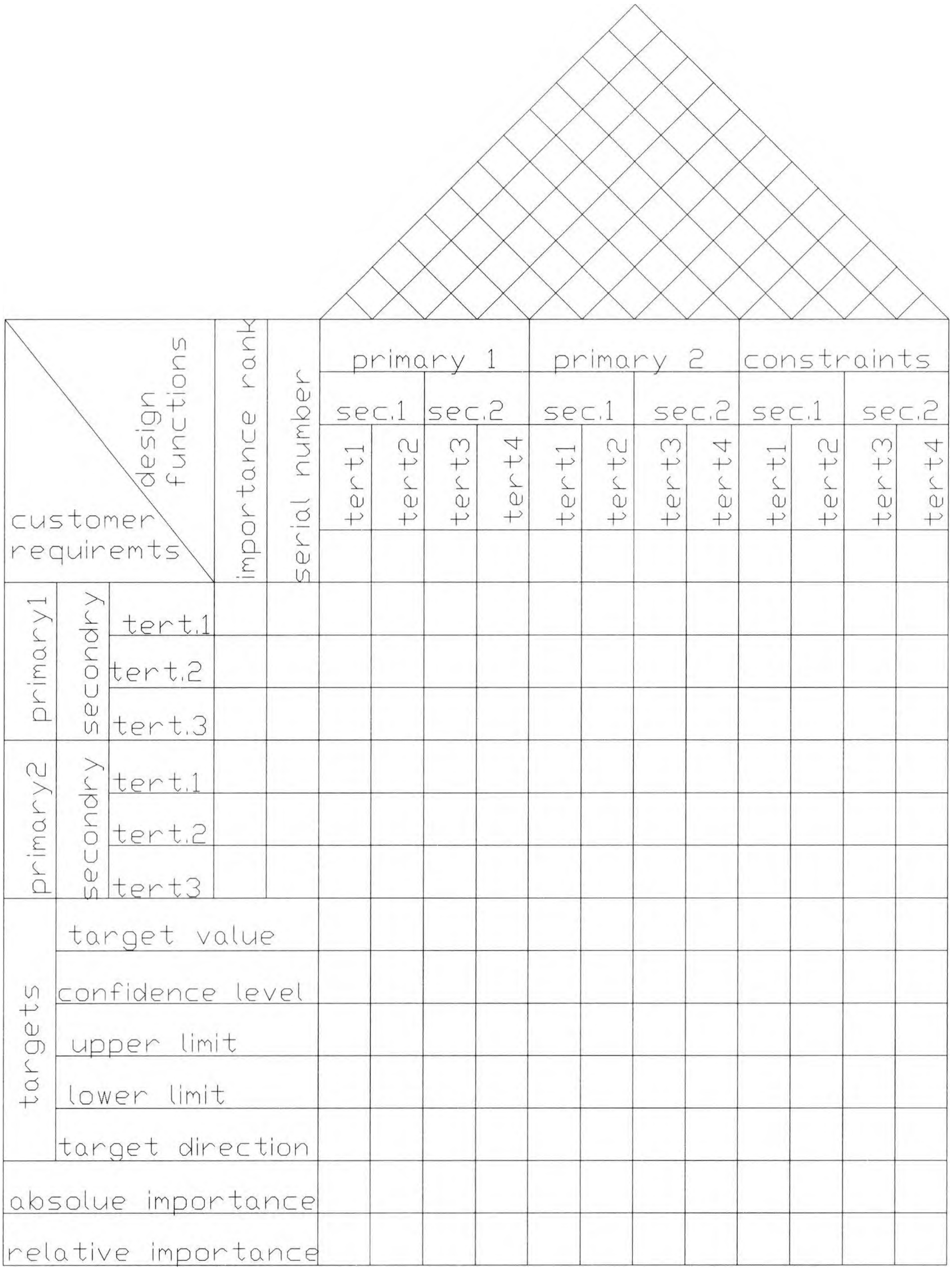


Fig. 3-5 Main DFD chart

3.5- CONCURRENT ENGINEERING

Before discussing concurrent engineering, it is useful to describe the traditional introduction and product development practice of the majority manufacturing companies. Typically, in a manufacturing organisation, marketing identifies the need for new products, price ranges and their expected performance from customers or potential customers.

As design is carried out in relative isolation, manufacturing, test, quality and service functions only see the design in an almost complete state. The process is done in a sequential progression, each state of product development follows completion of the previous stages. This is commonly known as '*over the wall*' engineering. In this sequential method of operation, a change required in a later stage will cause delay and additional costs in the upstream stages. Additionally, the subsequent stages will be delayed until the current stage has been completed. There are many weaknesses of over the wall engineering approach. In summary, they include:

(1)-Insufficient product satisfaction, leading to an excessive amount of modifications;
(2)-Little attention to manufacturability issues of the product at the design stage;(3)-The estimated costing is usually degrees of magnitude in error, due mainly to the uncontrolled late design change costs;(4)-The likelihood of late changes usually leads to expensive changes to tooling and other equipment.

Concurrent engineering provides a systematic and integrated approach to introduction and design of products. It includes design for manufacture, design for assembly, design for maintainability, design for cost effectiveness etc.

The design process is done in a continuous and complete information interchanging between different departments. The commencement of each distinct stage is not dependent upon full completion of the preceding stages; overlapping activities can take place, leading to concurrency in product development.

Concurrent design (or sometimes called parallel) is an approach, which specifies that all analysis be performed at once and any new design be based, not on the results of one analysis, but on the total analysis package. The prevalent design process today first examines and ensures conformance to functional performance constraints and then evaluates the part for manufacturability. In many cases, a functionally acceptable design will be found to be nonmanufacturable, and the designer must then redesign the part and re-analyse the functional characteristics before resubmitting to a manufacturing analysis. The parallel design concept includes manufacturability and, in fact, all pertinent analysis, to be performed on each design iteration simultaneously.

Tompkins [126] defines concurrent engineering as a parallel performance of product and process design. It is a considerable interaction between product and process design to insure the product is designed to be easily manufactured.

Youssef [138] views it as a design philosophy that promotes collective and integrated efforts of a number of teams involved in planning, organising, directing, and controlling all activities related to products and processes from idea generation to finished product.

Studies considering the cost associated to a product during its entire life cycle have demonstrated that from 60 to 95% of these costs are incurred during the design phase [119]. Therefore, it is during the design stage that the best savings can be achieved. Moreover the earlier the improvements are made the greater is the cost reduction.

The purpose of concurrent engineering is to ensure that the decisions taken during the design of a product result in a minimum overall cost during its life cycle. In other words, this means that all activities must start as soon as possible, to introduce working in parallel, which additionally shortens the overall product development, process.

As product life cycles decrease and manufacturers are faced with increasing global competition, engineering design plays an increasingly important role in the successful manufacture of products. It is increasingly difficult, not to mention undesirable, to consider products independent of process and customer needs; hence, the increasing emphasis on concurrent engineering as a critical systems integration strategy. Of key importance is that new products be designed to support efficient production. The most consequential efforts in this domain are design for manufacture and assembly (DFMA). To represent a broad variety of design considerations, Gatenby [58] generalises the entire family of related design strategies as DFX, where X can represent several issues such as cost, maintenance, mobility, etc.

As DFX strategies become more pervasive in use, it is common for product designers to consider process capability issues to determine whether or not a product can be manufactured or assembled at a specific process. Designers now realise that the most advanced engineering designs may be poor performers in manufacturing or assembly centres in which they are difficult or impossible to produce. Boothroyd [20] discuss ways in which DFMA is now being broadened to include consideration of the difficulty of manufacture for various parts and how it is helping to facilitate team work and simultaneous engineering.

Jebb [73] define concurrent engineering as a methodology which provides a means of performing several activities related to the design, manufacture, and stages of product life cycle in a simultaneous and integrated manner. Because design affects all subsequent activities in the product's life cycle and because product assembly has historically accounted for a high proportion of the costs associated with manufacturing, early tools to support concurrent engineering focus on assembly [111]. Boothroyd [20] introduced the concept of DFA as a tool to support product design for assembly. Other DFA systems that have subsequently evolved are discussed by Poli [106]. Funk [56] discusses the dramatic decrease in manufacturing costs possible through the application of DFA techniques.

A significant number of authors suggest that the implementation of concurrent engineering strategies is critical if a company is to remain competitive among world manufacturers. Wallach [126], Gunderson [64], Dahne [37] and Eversheim [48], all use concurrent engineering as a basis to develop a model and methodology to support the integration of design and process planning. Keys [80] and Taylor [123] suggest that process selection and process planning should be a component of product design.

Main objectives of concurrent engineering include:

-Decreased product development lead-time;
-Improved profitability;
-Greater competitiveness;
-Greater control of design and manufacturing costs;
-Close integration between departments;
-Enhanced reputation of the company and its products;
-Promotion of team spirit.

3.6- TAGUCHI TYPE EXPERIMENTAL DESIGN

Taguchi [121] is a Japanese engineer and statistician who became widely known in the west in the early 1980s when the Ford Supplier Institute began promoting his ideas. This organisation later became the Independent American Supplier (ASI), of which Taguchi became the executive director.

As a result of the ASI's efforts, the term 'Taguchi methods' is now a common use in industry, and is often applied very loosely to any industrial experiment with a statistical basis. The arrival of the 'quality movement' of the 1980s gave impetus to industrial applications of a range of well established statistical methods, including the design and analysis of experiments as well as the techniques which have come to be known as statistical process control (SPC).

Like SPC, Taguchi methods could legitimately be presented as part of the explanation for the extraordinary progress in quality improvement made by the Japanese. Although Taguchi's work is often obscure, at least in translation, it was clear from the beginning that the mathematical and statistical detail was there to support a general philosophy of quality improvement based on the need to reduce variation.

3.6.1- PLANNING AN EXPERIMENT

The engineering process can be viewed as a combination of designing and testing, which commonly are within a cycle of design, test, redesign, retest and so on. Whichever way designing and testing are combined, experiments of one sort or another need to be carried out. By 'experiments' we mean any test, evaluation or trial designed to evaluate a change, which requires the collection of data so that a prediction on the performance of the system can be made as to whether further redesign is needed.

It is usually possible with a properly planned experiment to interpret the data using only simple statistical methods and with out calling on the help of an expert statistician. Nevertheless, the ability to obtain knowledge from data is skill that must be developed, and one component of this skill is statistical thinking.

It is a normal procedure that changes are made to the design as the engineering process develops, based on the most recent test information available. In its worst scenario, the experimentation can mean changing one parameter at a time, while keeping everything else constant. This approach is often thought as the only way to measure precisely the effect of a certain design change. This is because some design changes may have a particular effect on the system that depends on how the system was configured when the test was made; but subsequent changes to other parameters may nullify or even reverse the effects. The knowledge gained will, therefore, be incomplete. This 'change one thing at a time' approach, however, is very costly. The alternative to it is to use statistically designed experiments to plan the programme of testing. Statistical design of experiments means making many design changes at once and conducting several tests and evaluations before decisions are taken as to what the next steps in the development process should be. First impressions of this idea may be that changing several things at once will make the situation worse, in the sense that it will be impossible to tell which changes made the difference to the performance of the design. However, with statistically designed experiments, these design changes are not just any design changes.

To run a statistically designed experiment, one has to identify several factors prior to experimentation. ‘Factors’ are defined as the parameters that we want to change in an experiment. The factors are given different values or possibilities which are termed as ‘levels’. For example, in a steel material heat treatment experiment, temperature, time, heating rate, cooling rate, and carbon content are regarded as factors and the values assigned to them as levels. Here we have five factors and a given number of levels depending how many different values we decide to assign the factors and conduct the tests. If we were to choose two levels for every factor we would have 32 test runs to make in the ‘change one thing at a time approach’. Alternatively, we can plan the experiment by changing three factors at a time in a patterned sequence. This will greatly reduce the number of test runs that need be conducted before knowledge of performance due to change of factor is achieved. Statistical figures alone, however, could be misleading and one needs to constantly incorporate the figures with basic engineering knowledge and common sense.

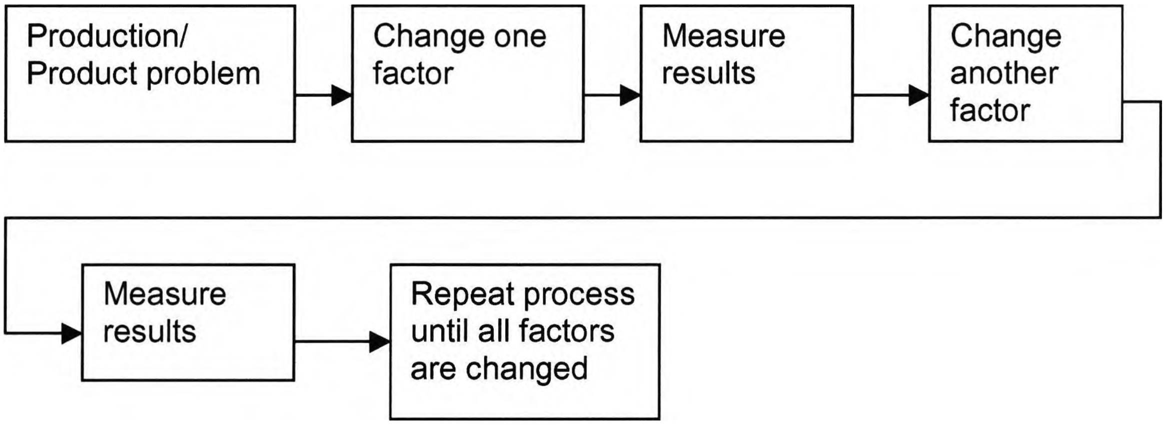
There might be occasions when one needs to study the effects of numerous multi-level sources. Prior experience and engineering judgement will then have to play a role in identifying those factors which are not expected to have a highly significant effect. The effects of these factors will be allowed to be ‘confounded’. Like the DFD methodology, the results are stored in tables for future use. Further experimentation should always be based on previous knowledge to screen out redundant or known design changes to reduce the number of test runs. After all, statistical thinking is aimed at reducing cost at the experimentation stage.

The performance of the engineering system is characterised by a measurement of some aspect of function. The quality measured in an experiment is called ‘response’. The response in the experiment above would be a combination of strength, hardness and/or ductility depending on what is required of the outcome.

At first sight, this type of experimentation seems confusing; but if the impact of each factor is evaluated in a proper statistical order, it could improve knowledge on performance and quality at a much lesser cost compared to the change one factor at a time approach.

To evaluate the effect of each factor, simply look at the average values of the quality characteristic (response) when that factor was at level one, and compare it with the average value of the quality characteristic when the factor was at level two etc. For this to have a meaning, the experimental plan needs to have a pattern or balance. i.e. the number of times the factors are changed has to be uniform.

One factor at a time approach



Same problem using Taguchi methods, parameter design

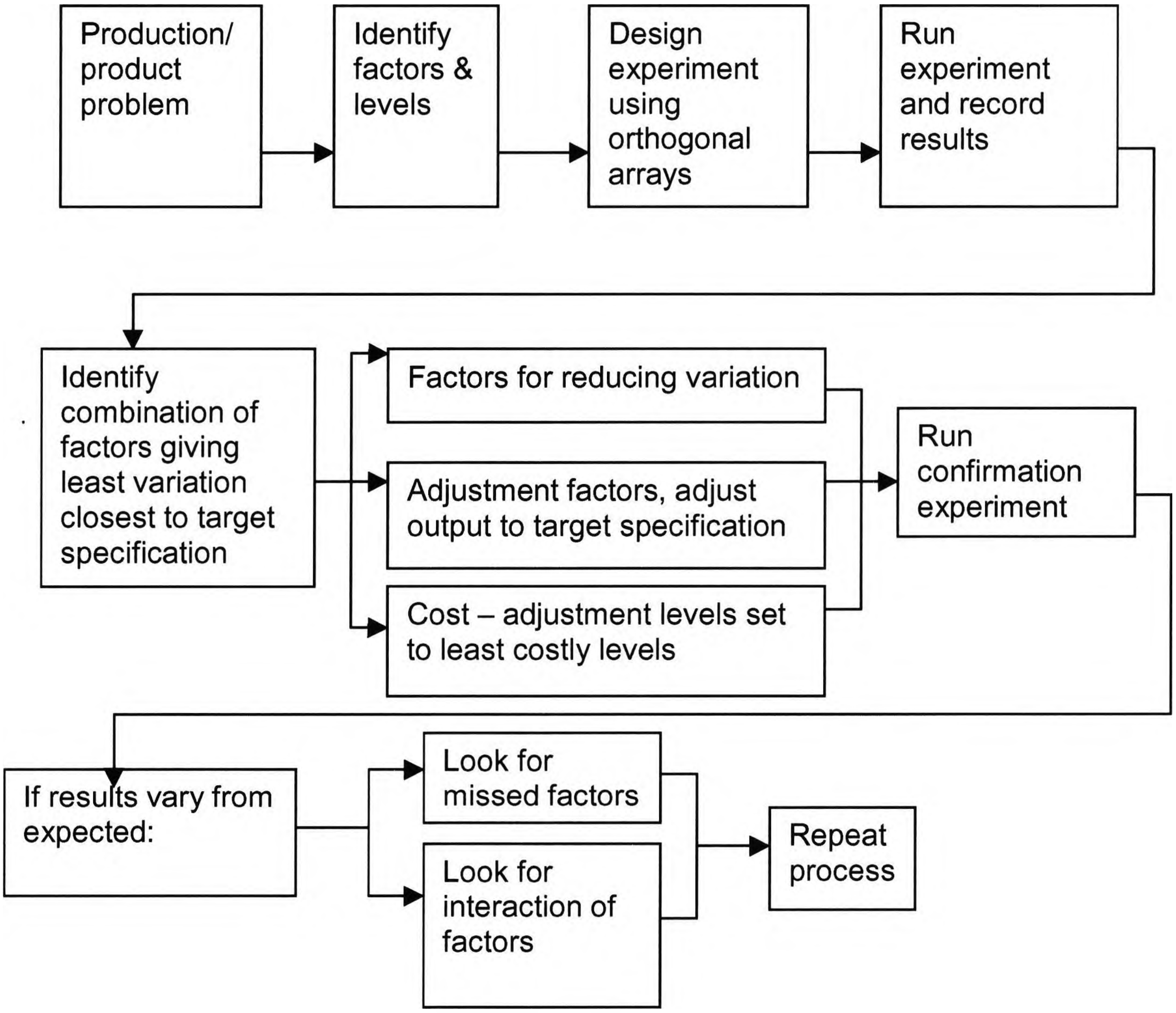


Fig. 3-6 Engineering problem solving methods

CHAPTER-4

DFD APPLIED TO SOFC DESIGN

4.1- INTRODUCTION

Design function deployment (DFD) methodology has been explored in detail in chapter three. It has been identified as a formal way to record the design process from an early stage of inception to the final stage of detailed design in a progressive manner.

In this chapter, DFD is applied into the design of solid oxide fuel cells (SOFC), starting with requirements identification through to the consideration of different conceptual designs, choice of materials, and fabrication techniques. All relevant data is recorded to ensure satisfaction of the specifications and for future reference. This is particularly important in the design of solid oxide fuel cells, as more follow up research and development is expected which is aimed at commercialisation of the product into the new millennium.

Entrance into manufacturing with absolute confidence of performance and market appeal is another important feature that can be exploited from design function deployment approach. Again, this enables to ensure that decisions are made after evaluating their cost implications. In an attempt to commercialise the solid oxide fuel cell technology, cost has proved to be the stumbling block. DFD divides the design procedure into parts to identify where the bottle-neck lies and attempts a solution. The most important feature of the design methodology in this application, however, is maximising knowledge about the cell performance at the design stage, which will minimise or eliminate down stream engineering changes, which in turn will reduce the cost.

The design process at different stages, is recorded in charts each containing all the relevant information at the particular stage.

4.2- CUSTOMER REQUIREMENTS

At this stage, a list of all requirements for the solid oxide fuel cell system are established. The list includes all customers ranging from the end user, manufacturing and assembly, financial and legal, environmental, and the company (designer). This is done without any reference to the degree of importance of the requirements. Customers' requirements are not necessarily clear to the designer at the initial stage. Nevertheless, requirements are recorded in the customers' own words for later analysis and deployment.

The requirements are categorised into four groups according to their relevance to the customer. These are general (Fig.4-1), design (Fig.4-2), legal (Fig.4-3), and manufacturing requirements (Fig.4-4). The general requirements, for example, are mainly those that appeal to the buyer or end user. Here, the customers list what they require of a functioning fuel cell. This could be in comparison to conventional power generators, like heat engine, or other types of fuel cells. The design requirements, on the other hand, are those that are listed by the designer or any one with the knowledge of fuel cell operations. These requirements are usually more technical than the corresponding general requirements. All the requirements including the manufacturing and legal are listed on the charts below.

The requirements, in this project, were not derived from customers directly. This won't be an easy task, as the solid oxide fuel cell is still under development. The product is not at a commercial stage yet; hence there is little knowledge about the product particularly from the end user's point of view. Developers like Siemens-Westinghouse, Rolls-Royce and British Gas have been looking at the prospects of such a technology as a potential contender for conventional power generators. Researchers have established the requirements for the product from different angles, in terms of cost, reliability, manufacturability, maintenance etc. When the product reaches a commercial stage, end users can be included through focus groups at the design stage. In this project, however, the requirements are confined to those presented in literature.

COST OF PRODUCT	cost of installation
	cost of running/power output
COMPACTNESS	total volume
	power/weight ratio
RELIABILITY	long term performance
	depreciation effect
MAINTENANCE	ease of maintenance
	cost of maintenance
START UP TIME	heating time
	power take off
EFFICIENCY	waste heat recovery
	power output/fuel consumption
CLEAN TECHNOLOGY	by-products
	noise pollution
OPERATIONS	control systems
	use environment
	mobile/stationary applications
PERFORMANCE	part load performance
	full capacity performance
	upgrading to larger capacity

Fig. 4-1 General customer requirements

MECHANICAL STABILITY	component thickness
	mechanical support
	size
	weight
THERMAL STABILITY	working temperature
	thermal strain
	thermal cracking
	differential expansion
CHEMICAL STABILITY	reducing environment
	oxidizing environment
	corrosion resistance
ELECTRICAL OUTPUT	current density
	voltage/cell
	active surface area
FAIL SAFE MECHANISM	series cell arrangement
	parallel cell arrangemewnt
MANIFOLD DESIGN	air/fuel barrier
	preheating mechanism
LOSSES	ohmic loss
	concentration polarization
	activation polarization
SEALING MECHANISM	sef sealing
	seal material
	differential expansion

Fig. 4-2 Design requirements

SAFETY IN PRODUCTION	chemical hazard
	respiratory irritants
SAFETY IN OPERATION	gas leakage
	noise and vibrations
	pollution
	protective conductors
	devices and insulators
SAFETY IN MAINTENANCE	

Fig. 4-3 Legal requirements

MASS PRODUCTION	total volume
	manufacturing rate
FABRICATION	materials
	fabrication technique
	geometry
	ease of fabrication
	cost of fabrication

Fig. 4-4 Manufacturing requirements

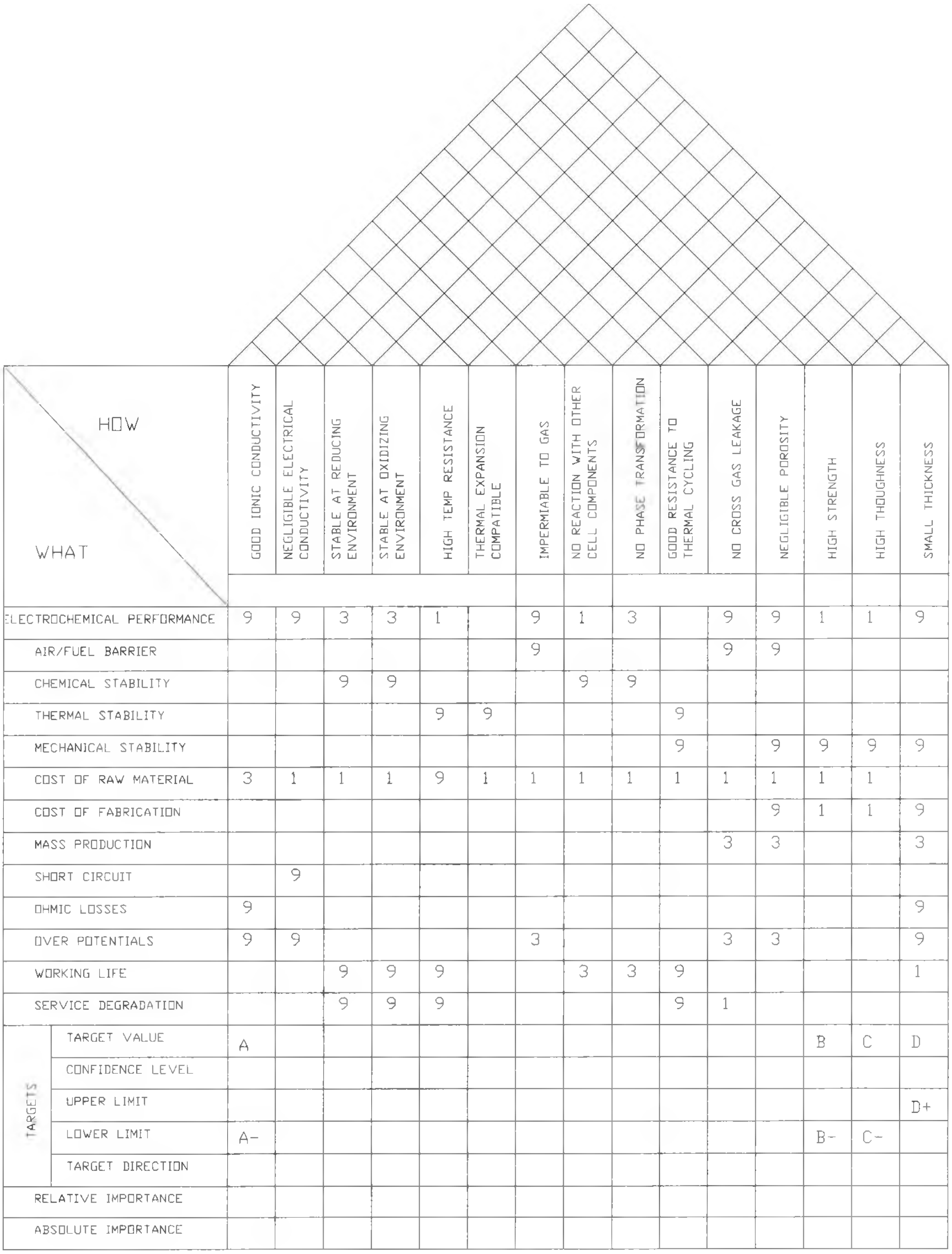
4.3- DESIGN FUNCTIONS

After careful analysis and overall consideration, the customer requirements for a solid oxide fuel cell are translated into functions in the designer's language in a solution neutral form. These design functions may, or may not, have numerical values attached to them. Here, the aim is to deploy all the requirements with one function or more. A matrix is then established showing the degree of relationships between the customer requirements and the design functions.

The relationships could be conflicting, where a certain design function is not good for a given requirement, or supporting where the function is an answer to the question. Whatever the case, the designer is only interested in the degree of relationships at this stage. Hence the relationship matrix alone is not a guide whether or not a requirement is fully deployed. A certain requirement could be related to one or more design functions. These functions, however, are not the final answer at this stage.

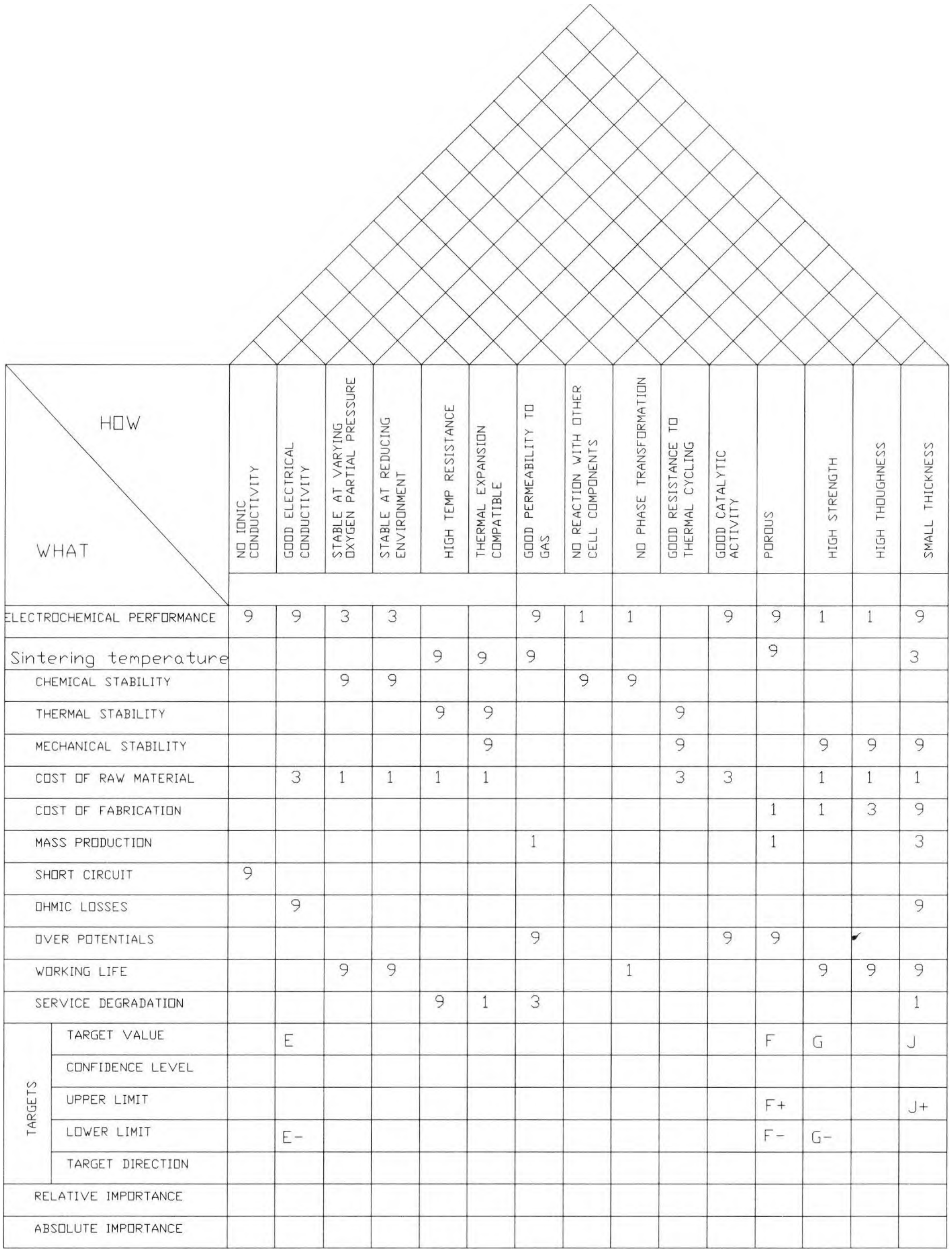
This matrix is designed to show, at first glance, whether or not deployment of the customer requirements is attempted. Most of the requirements are affected by more than one function. It is, therefore, important to establish how the functions affect one another. This will be left to the next stage, where the design function interactions are analyzed.

At this stage, the individual cell components are analyzed separately (Fig.4-5 to Fig.4-8). The first stage charts include, the customer requirements, the design functions and their relationships, and the *how much functions*. These are the upper limit, lower limit and the mean target values. The target information provides an objective assurance that customer requirements are met. It also serves as a yardstick for the design progress assessment and provides information for future improvement. The target values and directions of different variables determining the cell performance are recorded on the charts below.



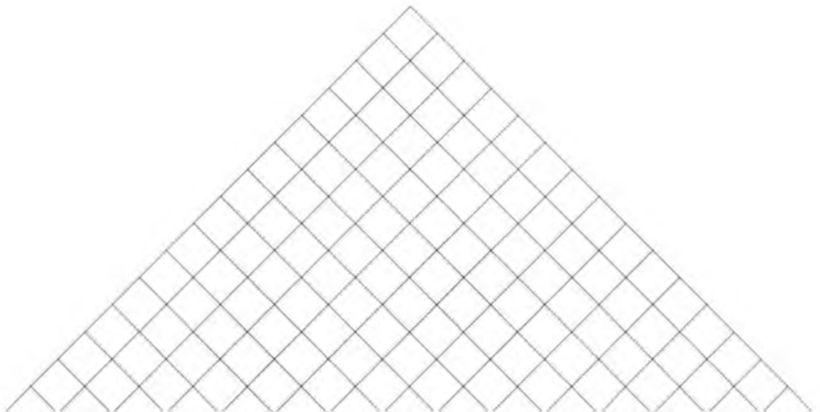
	HOW / WHAT	GOOD IONIC CONDUCTIVITY	NEGLIGIBLE ELECTRICAL CONDUCTIVITY	STABLE AT REDUCING ENVIRONMENT	STABLE AT OXIDIZING ENVIRONMENT	HIGH TEMP RESISTANCE	THERMAL EXPANSION COMPATIBLE	IMPERMIABLE TO GAS	NO REACTION WITH OTHER CELL COMPONENTS	NO PHASE TRANSFORMATION	GOOD RESISTANCE TO THERMAL CYCLING	NO CROSS GAS LEAKAGE	NEGLIGIBLE POROSITY	HIGH STRENGTH	HIGH THOUGHNESS	SMALL THICKNESS
	ELECTROCHEMICAL PERFORMANCE	9	9	3	3	1		9	1	3		9	9	1	1	9
	AIR/FUEL BARRIER							9				9	9			
	CHEMICAL STABILITY			9	9				9	9						
	THERMAL STABILITY					9	9				9					
	MECHANICAL STABILITY										9		9	9	9	9
	COST OF RAW MATERIAL	3	1	1	1	9	1	1	1	1	1	1	1	1	1	
	COST OF FABRICATION												9	1	1	9
	MASS PRODUCTION											3	3			3
	SHORT CIRCUIT		9													
	OHMIC LOSSES	9														9
	OVER POTENTIALS	9	9					3				3	3			9
	WORKING LIFE			9	9	9			3	3	9					1
	SERVICE DEGRADATION			9	9	9					9	1				
TARGETS	TARGET VALUE	A												B	C	D
	CONFIDENCE LEVEL															
	UPPER LIMIT															D+
	LOWER LIMIT	A-												B-	C-	
	TARGET DIRECTION															
	RELATIVE IMPORTANCE															
	ABSOLUTE IMPORTANCE															

Fig.4-5 Matrix for electrolyte requirements



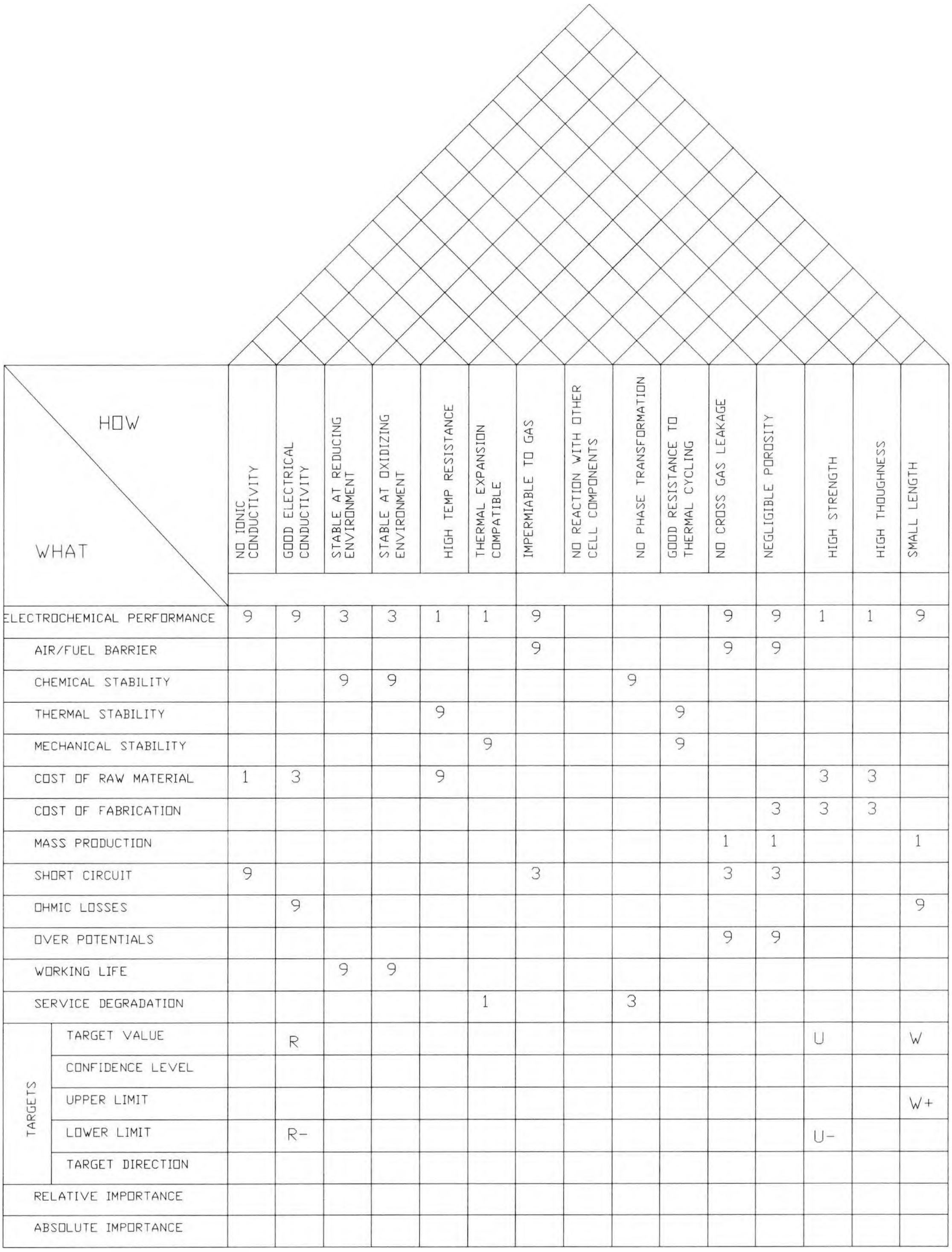
	HOW / WHAT	NO IONIC CONDUCTIVITY	GOOD ELECTRICAL CONDUCTIVITY	STABLE AT VARYING OXYGEN PARTIAL PRESSURE	STABLE AT REDUCING ENVIRONMENT	HIGH TEMP RESISTANCE	THERMAL EXPANSION COMPATIBLE	GOOD PERMEABILITY TO GAS	NO REACTION WITH OTHER CELL COMPONENTS	NO PHASE TRANSFORMATION	GOOD RESISTANCE TO THERMAL CYCLING	GOOD CATALYTIC ACTIVITY	POROUS	HIGH STRENGTH	HIGH THOUGHNESS	SMALL THICKNESS
	ELECTROCHEMICAL PERFORMANCE	9	9	3	3			9	1	1		9	9	1	1	9
	Sintering temperature					9	9	9					9			3
	CHEMICAL STABILITY			9	9				9	9						
	THERMAL STABILITY					9	9				9					
	MECHANICAL STABILITY						9				9			9	9	9
	COST OF RAW MATERIAL		3	1	1	1	1				3	3		1	1	1
	COST OF FABRICATION												1	1	3	9
	MASS PRODUCTION							1					1			3
	SHORT CIRCUIT	9														
	OHMIC LOSSES		9													9
	OVER POTENTIALS							9				9	9			
	WORKING LIFE			9	9					1				9	9	9
	SERVICE DEGRADATION					9	1	3								1
TARGETS	TARGET VALUE		E										F	G		J
	CONFIDENCE LEVEL															
	UPPER LIMIT												F+			J+
	LOWER LIMIT		E-										F-	G-		
	TARGET DIRECTION															
RELATIVE IMPORTANCE																
ABSOLUTE IMPORTANCE																

Fig.4-6 Matrix for cathode requirements



HOW / WHAT		NO IONIC CONDUCTIVITY	GOOD ELECTRICAL CONDUCTIVITY	STABLE AT VARYING OXYGEN PARTIAL PRESSURE	STABLE AT REDUCING ENVIRONMENT	HIGH TEMP RESISTANCE	THERMAL EXPANSION COMPATIBLE	GOOD PERMEABILITY TO GAS	NO REACTION WITH OTHER CELL COMPONENTS	NO PHASE TRANSFORMATION	GOOD RESISTANCE TO THERMAL CYCLING	GOOD CATALYTIC ACTIVITY	POROUS	HIGH STRENGTH	HIGH THOUGHNESS	SMALL THICKNESS
ELECTROCHEMICAL PERFORMANCE		9	9	3	3			9	1	1		9	9	1	1	9
Sintering temperature						9	9	9					9			3
CHEMICAL STABILITY				9	9				9	9						
THERMAL STABILITY						9	9				9					
MECHANICAL STABILITY							9				9			9	9	9
COST OF RAW MATERIAL			3	1	1	1	1				3	3		1	1	1
COST OF FABRICATION													1	1	3	9
MASS PRODUCTION								1					1			3
SHORT CIRCUIT		9														
OHMIC LOSSES			9													9
OVER POTENTIALS								9				9	9			
WORKING LIFE				9	9					1				9	9	9
SERVICE DEGRADATION						9	1	3								1
TARGETS	TARGET VALUE		K										M	N		Q
	CONFIDENCE LEVEL															
	UPPER LIMIT												M+			Q+
	LOWER LIMIT		K−										M−	N−		
	TARGET DIRECTION															
RELATIVE IMPORTANCE																
ABSOLUTE IMPORTANCE																

Fig.4-7 Matrix for anode requirements



WHAT	HOW	NO IONIC CONDUCTIVITY	GOOD ELECTRICAL CONDUCTIVITY	STABLE AT REDUCING ENVIRONMENT	STABLE AT OXIDIZING ENVIRONMENT	HIGH TEMP RESISTANCE	THERMAL EXPANSION COMPATIBLE	IMPERMIABLE TO GAS	NO REACTION WITH OTHER CELL COMPONENTS	NO PHASE TRANSFORMATION	GOOD RESISTANCE TO THERMAL CYCLING	NO CROSS GAS LEAKAGE	NEGLIGIBLE POROSITY	HIGH STRENGTH	HIGH THOUGHNESS	SMALL LENGTH
ELECTROCHEMICAL PERFORMANCE		9	9	3	3	1	1	9				9	9	1	1	9
AIR/FUEL BARRIER								9				9	9			
CHEMICAL STABILITY				9	9					9						
THERMAL STABILITY						9					9					
MECHANICAL STABILITY							9				9					
COST OF RAW MATERIAL		1	3			9								3	3	
COST OF FABRICATION													3	3	3	
MASS PRODUCTION												1	1			1
SHORT CIRCUIT		9						3				3	3			
OHMIC LOSSES			9													9
OVER POTENTIALS												9	9			
WORKING LIFE				9	9											
SERVICE DEGRADATION							1			3						
TARGETS	TARGET VALUE		R											U		W
	CONFIDENCE LEVEL															
	UPPER LIMIT															W+
	LOWER LIMIT		R-											U-		
	TARGET DIRECTION															
RELATIVE IMPORTANCE																
ABSOLUTE IMPORTANCE																

Fig.4-8 Matrix for interconnect requirements

Keys

9 = strong relationship
3 = medium relationship
1 = weak relationship

Target values

A = 0.15 $\Omega^{-1}cm^{-1}$	A- = 0.1 $\Omega^{-1}cm^{-1}$	
B = 300 Mpa	B- = 200 MPa	
C = 2.95 MPa $m^{1/2}$	C- = 1 MPa $m^{1/2}$	
D = 100 microns		D+ = 250 microns
E = 150 $\Omega^{-1}cm^{-1}$	E- = 50 $\Omega^{-1}cm^{-1}$	
F = 30%	F- = 20%	F+ = 35%
G = 40 Mpa	G- = 25MPa	
J = 20 microns		J+ = 50 microns
K = 500 $\Omega^{-1}cm^{-1}$	K- = 300 $\Omega^{-1}cm^{-1}$	
M = 30%	M- = 20%	M+ = 35%
N = 100 Mpa	N- = 75 MPa	
Q = 20 microns		Q+ = 50 microns
R = 30 $\Omega^{-1}cm^{-1}$	R- = 2 $\Omega^{-1}cm^{-1}$	
U = 150 Mpa	U- = 50 MPa	
W = 2cm		W+ = 3cm

Fig.4-9 Target values for the design functions.

The table in Fig.4-9, shows the target values that are assigned to the design parameters. These are the values for an acceptable fuel cell performance derived from mathematical models and experimental work carried out on the solid oxide fuel cell technology that is presented in literature [16,17,40,96]. The values will change with the development on the technology. For example, if cell component materials that operate at a lower temperature and with an equivalent conductivity to that of the current materials are discovered, the requirement on strength will be changed to a lower value as creep, corrosion and other problems associated with high operating temperature will be avoided.

4.4- INTERACTIONS

In a solid oxide fuel cell design, mechanical and electrical requirements are often in a direct conflict. This arises the need for a detailed interaction analysis between the two functions before attempting the trade off. The analysis is done in two steps. First, the nature and degree of interaction is established (Fig.4-10). This is followed by a conflict resolution exercise (Fig.4-11). It has been noted, in chapter-3, that it is necessary to try and make the trade off go away before attempting it.

The information is stored in the interaction table for future reference. As trade off is performed, certain functions that were meant to deploy requirements are eliminated. This affects the performance and/or quality of the final product. These charts are used to indicate where future research and development activities need be made to improve quality.

A lot of information in regards to the relationship between functions is stored in Fig.4-10. Some of the functions are supporting while others are in conflict with one another. The table is a reflection of the mechanical-electrical properties and requirements of cell components. More of a strong conflicting relationship between these properties can be seen in the table.

Ionic conductivity of YSZ electrolyte is acceptable for SOFC application at elevated temperature. At such temperatures, even microstructure (grain boundary) does not affect the conductivity significantly [96]. The conductivity is normally compromised with toughness. YSZ have been toughened by introducing inclusions of clinic Z_rO_2 that saw the conductivity to degrade to a level unacceptable for SOFC applications. Fine particles of partially stabilised Z_rO_2 and MgO additives have also been added to YSZ and without enormously affecting the ionic conductivity of the material while increasing the fracture toughens to compensate for the stress build up due to thermal expansion mismatch.

The cathode, having been exposed to the oxidant, is strongly affected by the degree of oxygen partial pressure. The lowest partial pressure before $L_aM_nO_3$ Cathode dissociates into multiple phases is termed as the critical oxygen partial pressure. At the same temperature, the critical partial pressure increases with increasing additives concentration. Thus a high additive content generally results in reduced stability for the cathode. Strontium and calcium additives are commonly used in SOFCs because $L_aM_nO_3$ doped with these dopants has high electronic conductivity in oxidising atmospheres and relatively matches the thermal expansion of other cell components.

The main problem with the anode material is the fact that it has higher thermal expansion coefficient than the rest. Additives are used to reduce it without causing the other properties, like conductivity, to deteriorate.

Previous research works have concentrated in finding alternative materials for the cell components especially in reducing the working temperature thereby reducing the conflicts between mechanical and electrical requirements. So far the materials that can be used for SOFC applications are limited due to the high working temperatures and prohibitive cost limitations. The solution oriented interaction chart in Fig.4.11 thus suggests the need for combining the different properties to suit the applications. That means a compromise between properties is essential, as eliminating one material and replacing by another is not easy due to the limitations.

The conflict between the mechanical and electrochemical requirements are best illustrated by the interaction between the strength and porosity. Young's modulus decreases with increase in porosity with a steep gradient as shown in Fig(7-12).

This deteriorates the bending rigidity of the component. The figures indicate how strongly the parameters interact with each other.

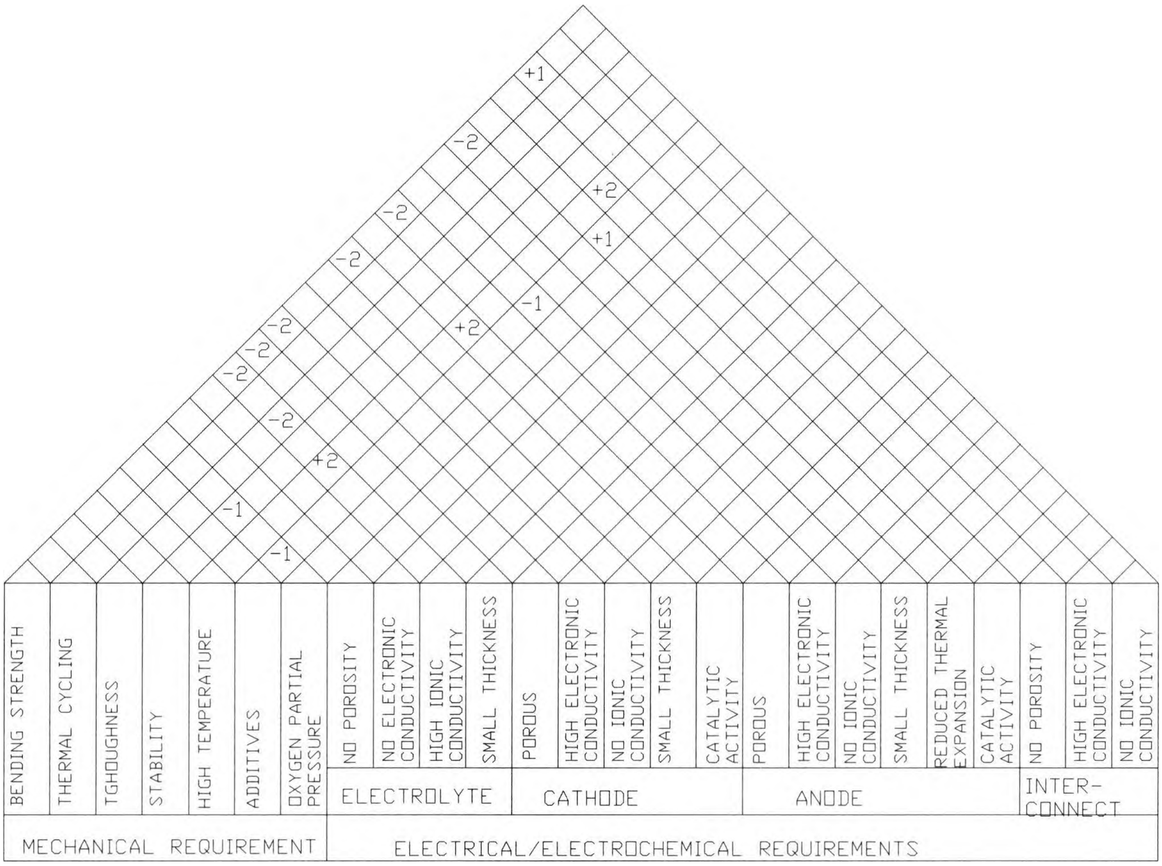


Fig.4-10 Mechanical – Electrical interactions (problem oriented)

Keys

-2 = strong negative
-1 = negative
+1 = positive
+2 = strong positive

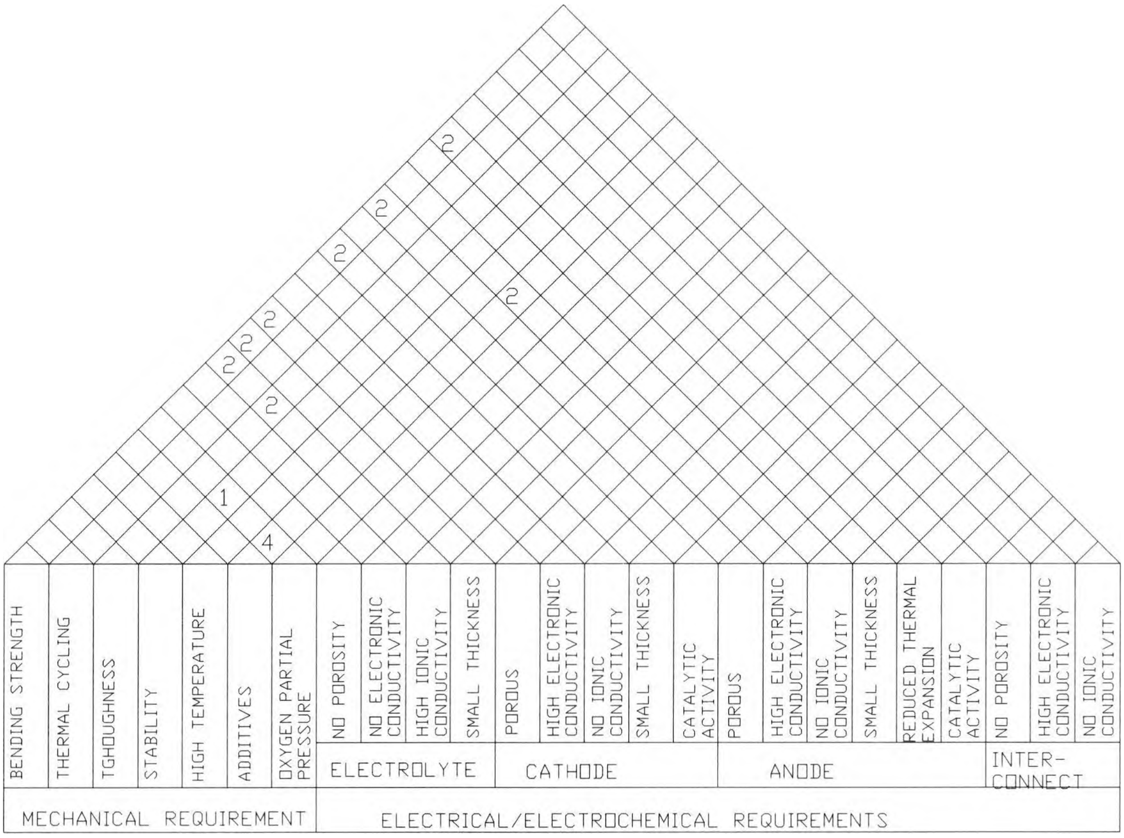


Fig. 4-11 Mechanical – Electrical interactions (Solution oriented)

Keys

1 = eliminate
2 = combine
3 = transfer
4 = modify

4.5- CONCEPTUAL DESIGNS

Different solid oxide fuel cell designs have been proposed over the years. Four of such conceptual designs were discussed in detail in chapter two. Some of the designs posses an advantage over others with respect to certain performance functions. Others might perform better in other areas of the design functions. To evaluate their performance qualitatively, all the designs are compared simultaneously under the same matrix.

The requirements are assigned with weighting factors depending on their importance to the customers and their effect to the overall quality. By quality, we mean the degree to which a product approaches the intended performance level. The weighting factors greatly depend on the products working applications. Power density, for example, might not be as important when the product is to be used as a power generator for an apartment compared to when it is used for space applications. In any case, the weighting factors as well as the performance rating are all recorded in a chart for future applications.

The design configurations of the four types that were discussed in chapter two and a new configuration proposed in this project are shown on (Figs 4-12 to 4-16). The new design configuration named, as a combined design is a configuration evolved from the previously proposed conceptual designs.

The different design concepts have their advantages and disadvantages compared to one another. So far, the tubular design (Fig.4-12) has been the most advanced of them all. It needs no gas seals, which would eliminate problems related to sealing. The fact that each cell is built as a unit structure minimizes the problem with cracking induced by thermal stress. As indicated in Fig (4-17), however, it has a long current path compared to the other cell configurations leading to higher ohmic losses. In this configuration the current path is long in the electrodes and short on the interconnect which results in an increased resistive losses. The support tube adds weight and reduces the power density. It also restricts the amount of oxygen transportation to the cathode.

The structural support is absent in the segmented-cell-in-series design (Fig.4-15) to give way to a better oxygen transportation and improved power density. This, however, does not come without cost. Cell components' thickness is compromised to be higher in order to accommodate a self-supporting mechanism, which in turn increases resistive losses. The current path can be made as short as possible to reduce resistive losses.

Another design with short current path is the monolithic design (Fig.4-13), which allows higher current density and less losses. It also posses a high power density and improved efficiency. Manufacturing the corrugated structure, however, remains difficult. Any significant thermal expansion mismatch can cause stress in the fired bodies and cause cracking in this design.

The planar (flat plate) design (Fig.4-14) offers flexible and simple cell geometry and is easier to fabricate. The cell components can be fabricated separately which makes possible multiple options of fabrication methods. Cell components can also be inspected for quality control individually. Due to the nature of their fabrication and assembly, planar SOFCs can readily incorporate different materials such as metallic interconnects. Sealing, however, is a great problem with this type of configuration.

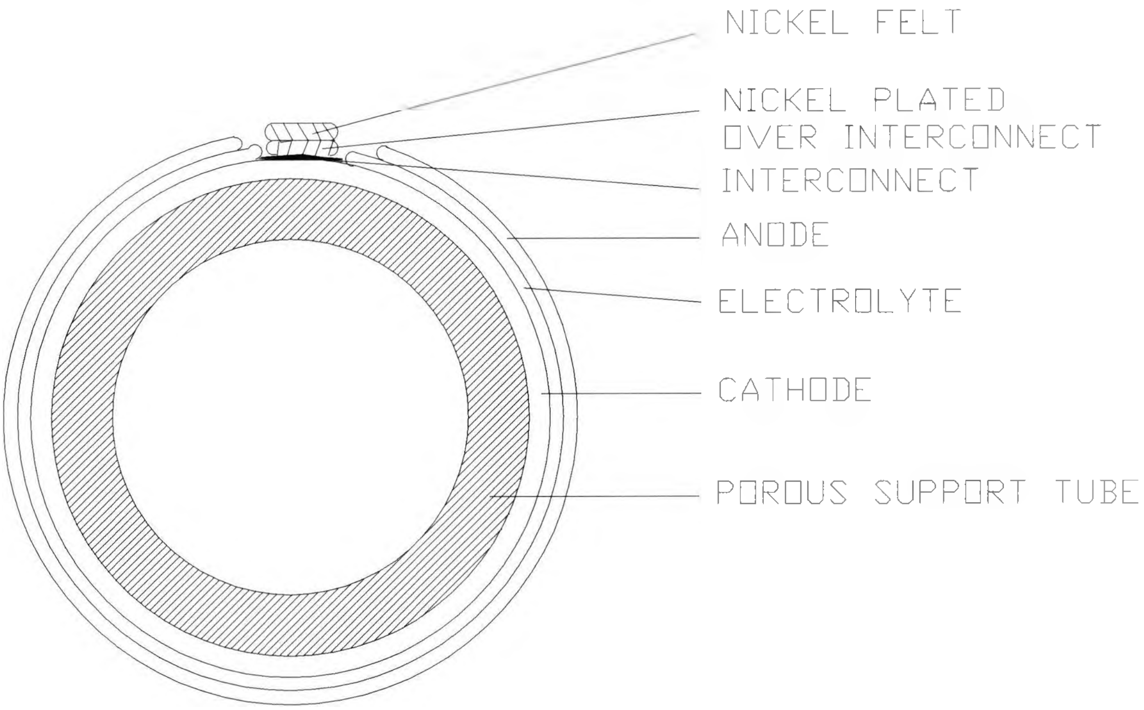


Fig.4-12 Tubular conceptual design

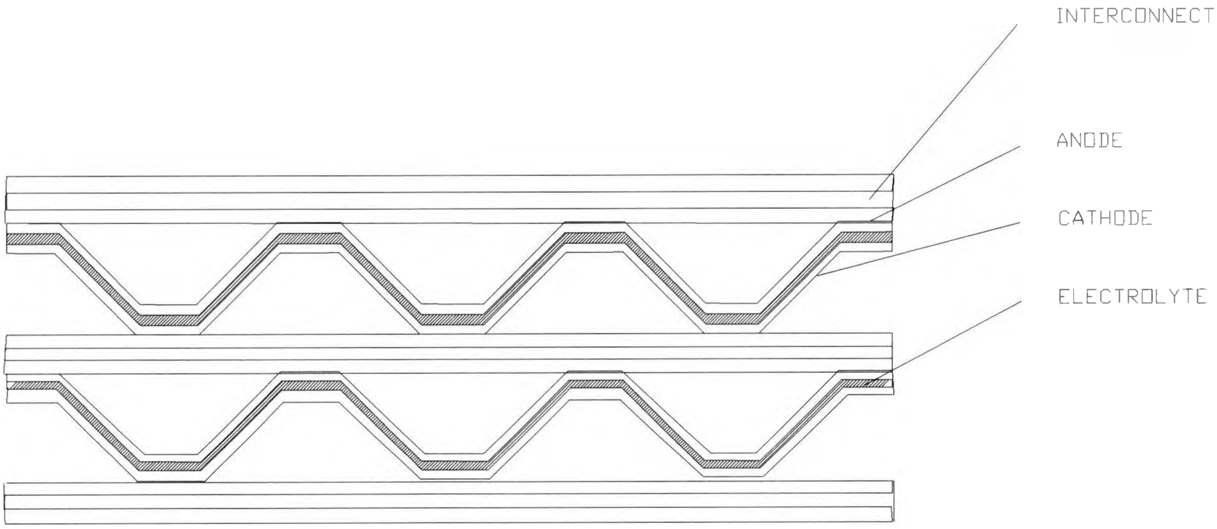


Fig. 4-13 Monolithic conceptual design

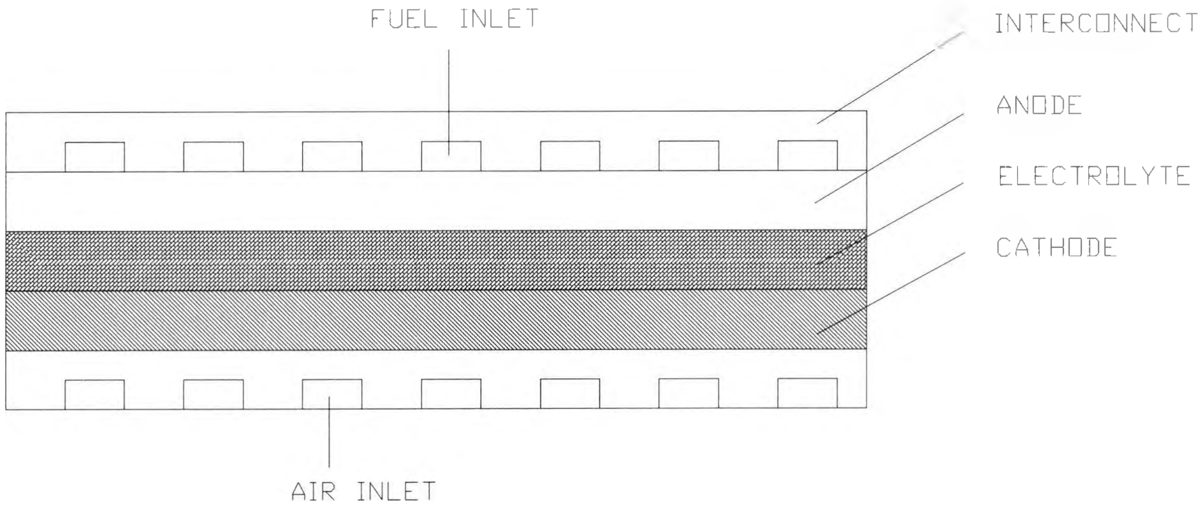


Fig. 4-14 Planar conceptual design

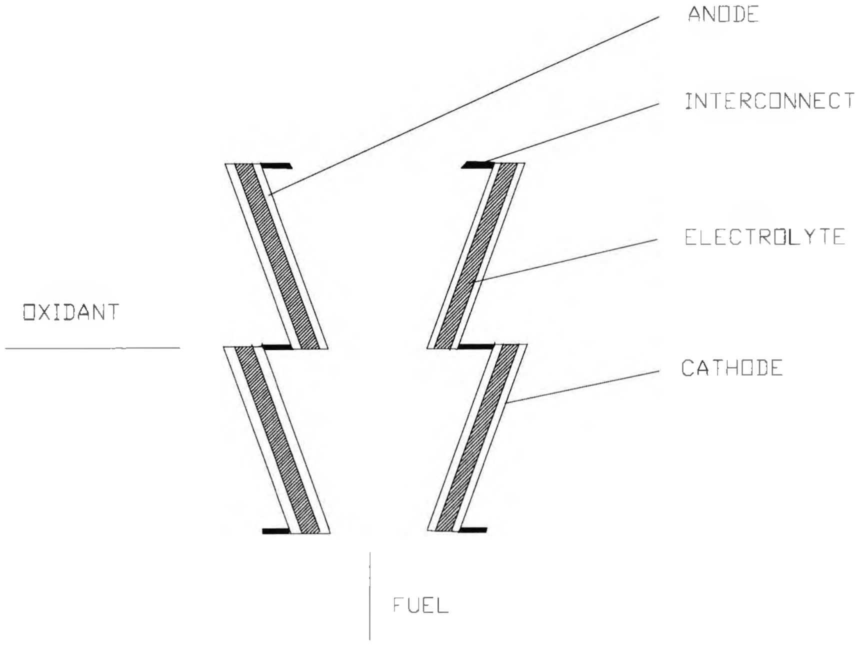


Fig.4-15 Conical conceptual design

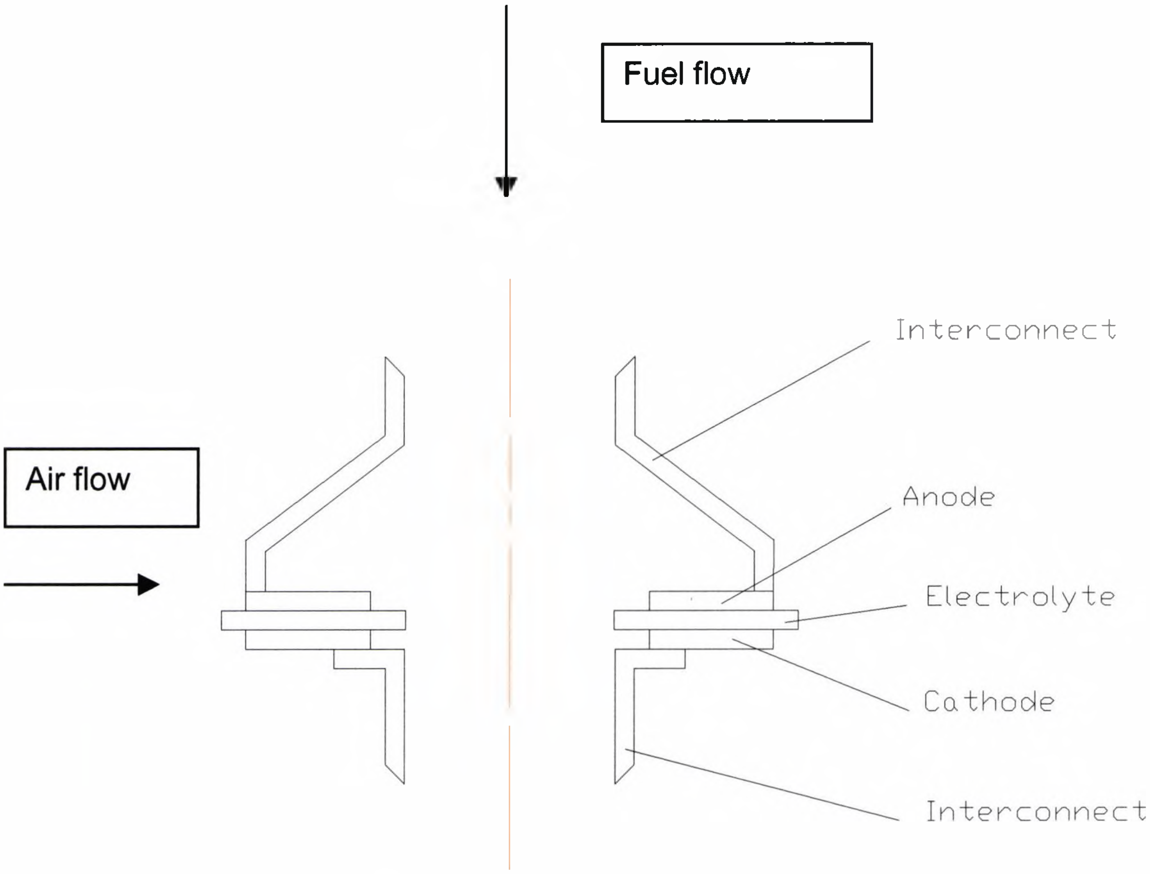


Fig.4-16 Proposed cell configuration

4.5.1 PROPOSED CONCEPTUAL CELL DESIGN

The combined configuration possesses all the advantages of a planar design with its circular flat plate electrolyte and electrodes (Fig.4-16). Sealing problem faced by the planar design is improved by the introduction of a tubular interconnect with the best of both worlds built into the design. This will, however, increase the current path but since the increase is on the interconnect and not electrodes, the resistive losses can be kept less than that of tubular. The figures in the decision matrix (Fig. 4-17) indicate that the combined cell configuration, which is introduced in this project, yields the best cell performance compared to the other configurations. The decision matrix is part of the DFD charts where the recorded requirements are taken as a yard-stick of comparison between the proposed conceptual designs where weighting factors are assigned to them depending on their importance. The weighting factors and scores assigned to the design functions and product performance respectively are only subjective. Care must be exercised in dealing with the figures in order to exploit the technique in achieving the optimum product design.

Cost of fabrication and manufacturing constraints associated with it played a dominant role in the decision-making process. The combined cell design with its advantage of planar components manufactured by press sintering technique and the quality control associated with that, combined with its tubular sealing mechanism was chosen to be the design for this application, despite the penalty on ohmic losses, which showed an increase to a specific resistance of 0.6 Ω-cm^2 compared to 0.4 Ω-cm for the planar design. The decision could, however, been easily different if the product was intended for space applications, where efficiency and power density would be the main requirements and cost would take a second place. This is a demonstration of why the weighting factors and scores are subjective that depend on factors like the intended application of the product. A detailed drawing of the combined design is presented in Appendix - A.

		CONCEPTUAL DESIGN CONFIGURATIONS									
		PLANAR DESIGN		MONOLYTHIC DESIGN		TUBULAR DESIGN		CONICAL DESIGN		COMBINED DESIGN	
	WEIGTING FACTOR	SCORE	WEIGHT	SCORE	WEIGHT	SCORE	WEIGHT	SCORE	WEIGHT	SCORE	WEIGHT
FABRICATION EASE	1.2	3	3.6	1	1.2	2	2.4	2	2.4	3	3.6
FABRICATION COST	1.2	3	3.6	1	1.2	1	1.2	2	2.4	3	3.6
POWER DENSITY	1	2	2	3	3	1	1	2	2	2	2
SEALING MECHANISM	1.2	1	1.2	2	2.4	3	3.6	2	2.4	2	2.4
DISSIPATIVE LOSSES	1	2	2	3	3	1	1	2	2	3	3
RESISTANCE LOSSES	1	1	1	2	2	3	3	2	2	1	1
EASE OF ASSEMBLY	1	3	3	2	2	2	2	1	1	2	2
CURRENT PATH	1	2	2	2	2	2	2	3	3	1	1
GAS MANIFOLD	1.3	1	1.3	2	2.6	3	3.9	3	3.9	3	3.9
CURRENT DENSITY	1	2	2	3	3	2	2	2	2	2	2
OUTPUT VOLTAGE	1	2	2	2	2	2	2	3	3	2	2
THERMAL EXPANSION RESISTANCE	1	2	2	1	1	3	3	1	1	2	2
QUALITY CONTROL	1	3	3	2	2	1	1	2	2	3	3
STRESS DISTRIBUTION	1	1	1	2	2	3	3	2	2	2	2
COMPACTNESS	1	2	2	2	2	3	3	2	2	2	2
RELIABILITY	1.1	3	3.3	2	2.2	2	2.2	2	2.2	3	3.3
TOTAL			35		33.6		36.3		35.3		38.8

Fig. 4-17 Decision matrix

Keys

3 = high score
2 = medium
1 = low score

The figures in Fig(4-17) show how decisions were made and what factors dominated the decision making process. This clearly shows the subjective elements of the design process to make a follow up design easy and less time consuming, which in turn contributes to the reduction of development cost.

4.6- MATERIAL SELECTION

In any design process, material selection, the associated manufacturing technique, and the cost are inseparable. This activity particularly plays a pivotal role in the design of solid oxide fuel cells. The high operating temperature limits the choice of materials suitable for the job. A search for alternative materials that would reduce the cost of material and fabrication is already underway.

The choice of fabrication technique depends greatly on the design configuration and geometry and vise versa. While choosing a viable design configuration with the commonly used materials is the objective of this project, finding a replacement for yittra-stabilized zirconia electrolyte by a reduced temperature oxygen-ion conductor is another area where further research is required. This would reduce material and fabrication problems and improve cell reliability during prolonged operation.

Much of the research is centred on a search for alternative electrolyte as it is the core of the cell and other cell components are made to be compatible with it. Fig (4-18) is a list of possible materials for solid oxide fuel cell components, and a comparison between them in reference to the required performances. Most of these materials fail to be realisable due to prohibitive cost and insufficient long-term stability. Thermal expansion compatibility is another important factor that needs to be taken into account. The effect of thermal expansion can vary from one cell configuration to the other. A carefully analysed geometric layout of cell components can be applied to compensate for thermal expansion and stress build up. The comparison matrix is based on the combined SOFC design configuration. The chart can also be used in the search for alternative materials for the cell components.

The materials of choice for the cell components are given rating values of 1, in the materials list matrix (Fig.4-19) followed by values of 2 and 3 to the less appropriate materials from the list. The chart serves as a comparison between materials as well as a record for future reference in the search for alternative materials.

					PERFORMANCE														
			SERIAL NUMBER	RATING	COST	FABRICABILITY	STRENGTH	TOUGHNESS	ELECTRONIC CONDUCTIVITY	IONIC CONDUCTIVITY	PARTICLE SIZE	PARTICLE SIZE DISTRIBUTION	AGGLOMERATE STRENGTH	THERMAL STABILITY	CHEMICAL STABILITY	THERMAL EXPANSION COMPATIBILITY	DEGREDATION AT SERVICE	OXYGEN PARTIAL PRESSURE RANGE FOR CONDUCTION	SURFACE TOLLERANCE
MATERIALS LAY OUT	ELECTROLYTE	PURE ZIRCONIA (ZrO_2)		3	2	2	2	2		3			3	3	3		3	3	
		YITTRA-STABILIZED ZIRCONIA ($ZrO_2-Y_2O_3$)		1	2	2	2	2		2			2	2	2		2	1	
		BISMUTH OXIDE (Bi_2O_3)		2						1				3	3			3	
		CERIA DOPED CALSIUM OXIDE (CeO_2-CaO)		2						2				3	3			3	
	CATHODE	LANTHANUM MANGANATE ($LaMnO_3$)		1	2				2						1	2			
		PLATINUM		3	3				1						2	3			
		LANTHNUM COBALTITE ($LaCoO_3$)		2	2				2						3	3			
		TIN DOPED IDIUM OXIDE (In_2O_3I)		2	3				1						2	2			
	ANODE	NICKLE CERMET		1	1	3			1			2			2	2			
		PLATINUM		3	3														
		PALLADIUM		3	3														
		COBALT		2	2	2			1			2			2	3			
	INTERCONNECT	LANTHANUM CHROMITE ($LaCrO_3$)		1					1						1				
		NICKEL		2					1						2				
		INCONEL		2					1						2				
	TARGETS	TARGET DIRECTION																	
		UPPER LIMIT																	
		LOWER LIMIT																	
		TARGET VALUE																	
		CONFIDENCE																	
	RELATIVE IMPORTANCE																		
	ABSOLUTE IMPORTANCE																		

Fig. 4-18 Cell materials matrix

Keys

1 = good   2 = medium   3 = bad

4.7- DESIGN ANALYSIS

Mathematical models along with a statistically designed experimentation were used to maximize knowledge on the performance of the fuel cell before decisions are made. This is aimed at getting the design right the first time round. It is an extension of the Robust Engineering approach introduced in chapter three.

The computational models and the experimentation are all interdependent. Fig. 4-19 shows the relationship between the design variables and the models developed. Rate of air/fuel flow, for example, is dictated by electrochemical requirements (i.e., the supply of fuel and oxidant to the reaction sites) and by circulation requirements. These are answered on the electrochemical model and fluid flow model respectively. Another example, which is of utmost importance, is porosity. This is the variable where the trade off between electrical and mechanical requirements is centred. Its lower limit, for the electrodes, is dictated by the air transport (diffusion to the reaction sites) requirements while its upper limit is dictated by mechanical stability requirements. Hence porosity is analysed for gas transportation on the electrochemical model, mechanical stability on the thermal stress analysis model, and its level depends on the densification analysed on the experimental stage.

The models are designed in such a way that output data from one is input on the other in a form of a loop to find optimum fuel cell operating conditions. This calls for the need of an optimisation technique to integrate the mathematical models into the design process. Each mathematical model and experimental analysis are discussed in subsequent chapters in detail.

	ELECTROCHEMICAL MODEL	THERMAL STRESS MODEL	FLUID FLOW MODEL	TAGUCHI EXPERIMENTAL DESIGN
CELL CONFIGURATION	*	*	*	*
CELL THICKNESS	*	*		*
CELL DIAMETER	*			
STACK LENGTH				
MANIFOLD DESIGN			*	
AIR FLOW RATE			*	
FUEL FLOW RATE	*		*	
FUEL UTILIZATION	*			
CURRENT DENSITY	*			
VOLTAGE OUTPUT	*			
SINTERING TIME				*
SINTERING TEMPERATURE				*
COMPACTION FORCE				*
POROSITY LEVEL	*	*		*
STRESS DISTRIBUTION		*		
TEMPERATURE DISTRIBUTION		*		

Fig. 4-19 Matrix of mathematical models

4.8- BENEFITS OF THE DFD METHEDOLOGY

The use of DFD in the design of solid oxide fuel cells has been as a focussing aid where the customer requirements are given ratings and affect the decision making process depending on their importance. A case in point is the role of the manufacturing constraint identified during experimentation and the ease of fabrication of the planar cell components to dictate the choice of the design.

Much of the information can be efficiently retrieved and complete experience can be made available to future designers for further developments or modifications based on full knowledge of past experience. With the research and development on possible ceramic fuel cell components, many down stream design changes are inevitable. Experience gained here can readily be available for use through the DFD charts.

4.9- LIMITATIONS OF THE DFD METHODOLOGY

In this chapter, it has been shown that the DFD methodology can be particularly useful in selecting the best conceptual design by virtue of its facility for giving a thorough consideration to all the design requirements.

Typically a triangular matrix is used as the roof of the DFD charts. This matrix is used to identify which design parameters interact with each other and declare whether the interactions are supporting or conflicting. These interactions have implication for the optimisation goal in a multi-objective design problem. Each parameter is given target values and improvement directions. This matrix, however, fails to indicate the direction of influence between parameters. In the numerical optimisation stage, some parameters are given trial numerical values and others calculated until an optimum solution is achieved. Using the existing DFD methods, deriving parameter values from other set of parameters is not easily performed, as there is no indication of a hierarchy of parameter determination. In other words, present DFD methodology is not ideal when it comes to integrating mathematical results into the design procedure. In chapter 9, the DFD methodology is taken a step further to devise a way to decompose the correlation matrix into groups of variables with strong intra-group interactions and weaker inter-group interactions.

CHAPTER-5

Numerical simulation of air flow round the stack geometry

5.1- INTRODUCTION

If one were learning fluid dynamics as recently as 1960, one would have been operating in the 'two-approach world' of theory and experiment. However, the advent of the high-speed digital computer combined with the development of accurate numerical algorithms for solving physical problems on these computers has revolutionised the way we study and practice fluid dynamics today. It has introduced a fundamentally new third approach in fluid dynamics- the approach of computational fluid dynamics (CFD). Though CFD is no replacement for experimentation, it is an important design tool for modelling fluid flow in geometries (ranging from simple to complex) and optimisation prior to building a prototype.

In this chapter, a numerical analysis is presented of the air flow around the cell stack at different dimensional geometries and varying conditions. The predicted results are combined with the results of electrochemical and thermal models. Boundary layer effects are also analysed and optimum operating conditions determined. The calculations have been carried out on a proposed geometric design and a temperature of 1000^{o}c as the boundary conditions.

The problem is treated as a two dimensional, though the use of symmetry planes means that a three-dimensional problem, uniform in the k-direction is solved. Because of the symmetrical nature of the geometry and given boundary conditions, no change of variable occurs in the k-direction. This reduces the need for a great deal of time and computer memory.

5.2- GOVERNING EQUATIONS

The fundamental equations of fluid dynamics are based on the universal laws of conservation of mass, momentum (Newton's second law), and, in a non-isothermal flows, energy (first law of thermodynamics). Applying these conservation laws to a fluid flow, the continuity equation, the momentum equations, and the energy equation are derived. For unsteady, compressible flow, these equations are written, using an Eulerian approach and a vector notation as follows [124]:

(a) continuity equation

$$\delta\rho/\delta t + \nabla \cdot (\rho u) = 0 \qquad [5\text{-}1]$$

Where ρ is the fluid density, u is the fluid velocity vector and t is time;

(b) Momentum equation

$$\frac{\partial(\rho u)}{\partial t} + \nabla \bullet (\rho u \otimes u) = B + \nabla \bullet \sigma \qquad [5\text{-}2]$$

Where B is the body force and σ is the stress tensor;

(c) Energy equation

$$\frac{\partial(\rho h)}{\partial t} + \nabla \bullet (\rho u h) - \nabla \bullet (\lambda \nabla T) = \frac{\partial p}{\partial t} \qquad [5\text{-}3]$$

Where h is enthalpy, λ is thermal conductivity and p is pressure.

The main advantage of using a vector notation is that the equations apply to any co-ordinate system. All the equations above with five variables u, ρ, p, t, h are completed by the equation of state where:

$$\rho = \rho(T,p), \qquad [5\text{-}4]$$

$$h = h(T,p)\ . \qquad [5\text{-}5]$$

The transport equations are, therefore, summed over, using a Cartesian co-ordinate system as:

$$\frac{\partial \rho}{\partial t}+\frac{\partial(\rho u_i)}{\partial x_i}=0 \qquad [5\text{-}6]$$

$$\frac{\partial(\rho u_k)}{\partial t}+\frac{\partial(\rho u_i u_k)}{\partial x_i}=B_k+\frac{\partial \sigma_{ik}}{\partial x_i} \qquad [5\text{-}7]$$

For a Newtonian fluid, the stress tensor is given as:

$$\sigma_{ij} = -p\delta_{ij} + \mu' s_{kk}\delta_{ij} + 2s_{ij}\mu \qquad [5\text{-}8]$$

Where δ is Kronecker delta, μ is the coefficient of dynamic viscosity of the fluid and, μ' is its second coefficient of viscosity. S_{ij} is the strain rate tensor defined as:

$$S_{ij}=\frac{1}{2}\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right) \qquad [5\text{-}9]$$

The two coefficients of viscosity are related to the coefficient of bulk viscosity k by the expression,

$$K = 2/3\mu + \mu' \qquad [5\text{-}10]$$

Because the coefficient of viscosity is negligible except in the study of shock waves, the second coefficient of viscosity becomes,

$$\mu' = -2/3\mu \qquad [5\text{-}11]$$

And the tensor stress may be written as:

$$\sigma_{ij} = -p\delta_{ij} + u(2s_{ij} - 2/3s_{kk}\delta_{ij}) \qquad [5\text{-}12]$$

Substituting equation 8 into equation 5, the famous Navier-Stokes equation is obtained.

$$\frac{\partial(\rho u_j)}{\partial t}+\frac{\partial(\rho u_i u_j)}{\partial x_i}=B_j-\frac{\partial p}{\partial x_j}+\frac{\partial}{\partial x_i}\left\{u\left[\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}-\frac{2}{3}\delta_{ij}\frac{\partial u_k}{\partial x_k}\right]\right\} \qquad [5\text{-}13]$$

The Navier-Stokes equation can exhibit different mathematical characteristics, depending on the nature of the particular problem. They may represent a parabolic, hyperbolic or elliptic set of equations, or they can be a mixed set of those. The unsteady incompressible Navier-Stokes equations are a mixed set of elliptical-parabolic equations where the unknowns are the velocity vector u and the pressure p.

5.3- CFDS-FLOW3D: CODE OVERVIEW

CFDS-FLOW3D, also known as HARWELL-FLOW3D upto few years ago, is a general purpose thermofluid-dynamic computer code born, as other computer codes of the same family, in the early seventies and developed from a research work at Imperial College. Its original version was limited to simple staggered and rectangular grid, Cartesian or cylindrical co-ordinates. Since then a lot of improvements have been made. The current release CFDS-CFX4 is being used in this research work and also by the mechanical and aeronautical research groups at City University. Details presented below relate to this latest version.

The suite of CFDS programs consists of a number of modules:

(i) Pre-processing modules, or geometry and grid generators;
(ii) Interactive Frontend;
(iii) Frontend module of CFDS-FLOW3D;
(iv) Solution module of CFDS-FLOW3D;
(v) Post processing, or graphics modules.

The geometry and grid generators may be used to define the finite difference grid. The grid co-ordinates are dumped to a disk in a form readable by the Frontend. Though the use of a flag in the Frontend, the program is informed that the grid information is to be read in from disk. Use of these modules is optional. The grid can also be defined within the Frontend. The geometry and grid generators include the interactive grid generator, SOPHIA, which may also be used to specify some of the topological features of the geometry.

The Frontend takes input specification of the problem and converts it from a format convenient for the user to a one designed for efficient execution. Detailed error checking is performed. Facilities are available to provide a database, which calculates the physical properties of some common fluids, like air and water, termed as standard fluids. The problem is specified in a single data file using the Command Language, that is a set of English-like commands, subcommands, and associated keywords. In the interactive

Frontend, this data file is constructed automatically via a series of displays on the screen. User-defined Fortran routines may be included for features that are too complex to be described using the command language.

The solution module solves the discretized representation of the problem. It receives the information in a form that permits maximum efficiency to be obtained on different types of computers including vector processors. The solution module has only a few output facilities- for example, for printing and dumping the solution to the disk files.

The graphics modules produce the main graphics output, interrogating the disk files written by the solution module. Interfaces to other post processing packages have been constructed, and there are a number of post-processing options available for various workstations. Use of these modules is optional, and is described in the Environment User Guide.

In this research work, the interactive grid generator (SOPHIA) is used to define the geometric boundary condition and the finite difference grid. Problem specifications were made using the command language file. Calculations for local velocity vectors, pressure, and shear stresses were also carried out using the user subroutine USRTRN. The output produced was then used by the graphics packages to plot velocity patterns, or any other solution variables like pressure distribution across the geometry.
The main features of the command file and capabilities of CFDS-FLOW3D are given below.

Physical models and geometry

Physical space co-ordinates: Cartesian / cylindrical

Type of flow	laminar / turbulent
	steady / unsteady
	two-dimensional / three-dimensional
	incompressible / compressible
	isothermal / non-isothermal
	forced convection / natural convection
	buoyant: Boussinesq approximation / fully compressible
	multi phase flow: multi fluid model / homogeneous model
Boundary conditions:	solid walls
	symmetry or periodicity surfaces
	inlet / outlet faces
	pressure boundary
	mass flow boundary
Turbulence model:	κ-ε for high Reynolds number /
	low Reynolds number model
	high order turbulence models:
	algebraic Reynolds stress model /
	differential Reynolds stress model /
	differential Reynolds flux model
Combustion models:	two gaseous models:
	eddy break-up model /
	mixed-is-burnt model
Particle transport model:	Langragian
Grid:	rectangular / body fitted
	multi-block
	rotating co-ordinate system
	adaptive grids

5.4- CFD ANALYSIS

Three mathematical concepts are useful in determining the success or otherwise of CFD algorithms: convergence, consistency and stability. **Convergence** is the property of numerical method to produce a solution which approaches the exact solution as the grid spacing, control volume size or element size reduced to zero. **Consistent** numerical schemes produce systems of algebraic equations which can be demonstrated to be equivalent to the original governing equations as the grid spacing tends to zero. **Stability** is associated with damping of errors as numerical method proceeds. If a technique is not stable, even round off errors in the initial data can cause wild oscillations or divergence.

Performing the actual CFD computation itself requires operator skills of a different kind. Specification of the domain geometry and grid design is the main task at the input stage and subsequently the user needs to obtain a successful simulation result. The two aspects that characterise such a result are convergence of the iterative process and grid independence. The solution algorithm is iterative in nature and in a converged solution the so-called residuals-measures of the overall conservation of the flow properties are very small. Progress towards a converged solution can be greatly assisted by careful selection of the setting of various relaxation factors and acceleration devices. There are no straightforward guidelines for making these choices since they are problem dependent.

There is no formal way of estimating the errors introduced by inadequate grid design for a general flow. Good initial grid design relies largely on an insight into the expected properties of flow. A back ground in the fluid dynamics of the particular problem certainly helps and experience with gridding of similar problems is also valuable. The only way to estimate errors due to the coarseness of grid is to perform a ‘grid dependence study’, which is a procedure of successive refinement of an initially coarse grid until certain key results do not change. Then it can be concluded that the simulation is grid independent.

Numerical predictions of a flow are by no means conclusive on their own. An experimental data of some sort is normally used to back up and validate the computational results. It is not the purpose of this model, however, to establish the degree of accuracy of the predictions. The aim, here, is simply to maximise the knowledge of performance at the design stage. Again, in line with the design function deployment (DFD) methodology. The convergence of the residuals-measures, like mass, are a guide to the flow pattern to an acceptable accuracy, though not necessarily an accurate velocity/pressure distribution.

5.5- COMPUTATIONAL GRID AND GENERATION TECHNIQUES

One of the main problems in computing numerical solutions using finite element analysis is the generation of mesh for the solution domain. The grid has to be well-constructed; otherwise it might lead to an instability or lack of convergence. Numerical grid generation has now become a fairly common tool in the numerical solution of fluid flow problems.

Body-fitted curvilinear co-ordinate system- used in modern CFD codes- generated to maintain co-ordinate lines coincident with the boundaries were introduced to extend the capabilities of the FEM to deal with complex geometries and assist in the imposition of boundary conditions without the need of special procedures at the boundaries. The numerically- generated grid allows all computations to be done on a fixed square grid in the computational field, which is always rectangular by construction. However, the cost of greater flexibility afforded by the use of body-fitted grids and general co-ordinates is an increase in complexity of the equations to be solved, due to the non-linear co-ordinate transformation.

The first stem in the generation of the grid is the transformation of the physical space (complex geometry) into a computational domain (simple rectangular domain), where all numerical algorithms, like finite element, are implemented.

5.6- MANIFOLD GEOMETRY

In order to perform a fluid flow analysis on the fuel cell stack design, first we need to describe the flow geometry. Two manifold designs are proposed and analysed in this section. The first design, as shown in the Fig.5-1, consists of two 'L' shaped, concentric rectangular channels. Air is pumped in through the top end of the inner rectangular channel to be heated to a temperature of 1000°c, by the burner placed at the corner. The hot gas then exits to the bigger channel to heat up the cells to the required temperature. It eventually goes to the exhaust to complete the cycle, while heating the incoming cold air. The fuel is totally separated from the air and flows across the channel inside the cell stack. Initially the study is confined to the air/gas flow round the stack. The oxygen consumption in the electrochemical process is ignored as it is minimal compared to the volume of airflow. The second manifold design is more compact, where the stacks are arranged in a circular pattern that are equidistant from the heat source. Pre-heated air enters through the inner tube (Fig.5-2) to be heated by a ring burner and circulate around the stacks before exiting via the bigger channel. The schematic diagrams of the two conceptual manifolds are given below. The detailed drawing of which are also presented in the appendix. Half section of the manifold is considered for analysis due to symmetry.

5-7 RESULTS AND DISCUSSION

The fluid flow pattern analysis (Fig.5-4 & Fig.4-6) helps determine the manifold geometry. The over all flow field is simplified for analysis. A 2D flow pattern for both the designs are presented (Fig.5-1 & Fig.5-2). Test runs were made at different speeds and dimension of the geometry in order to arrive at an acceptable flow pattern. Here, the aim is not calculating pressure-velocity parameters, which is rather complex, if the 3D geometry along with the heat transfer factors were considered. Instead, a simplified 2D fluid flow pattern is determined to guide the dimension of the manifold design.

The second manifold design (Fig.5-2) possesses advantage in that it is more compact. The cells are placed equidistant from the heat source, which results in a uniform temperature distribution among the stacks. This is difficult to achieve in the L shaped design as the stacks are lined in the airflow path, some of which are too far from the heat source.

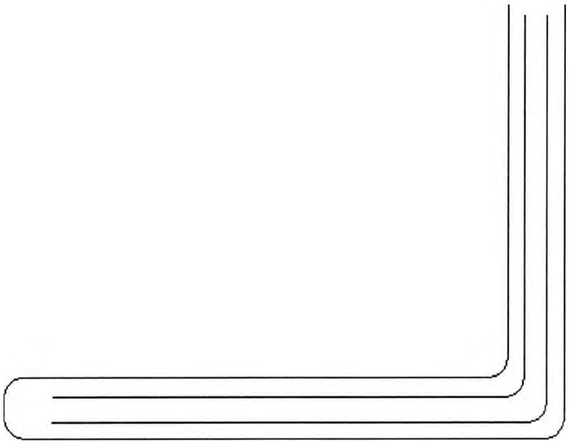


Fig.5-1 2D simplification of the L shaped manifold design.

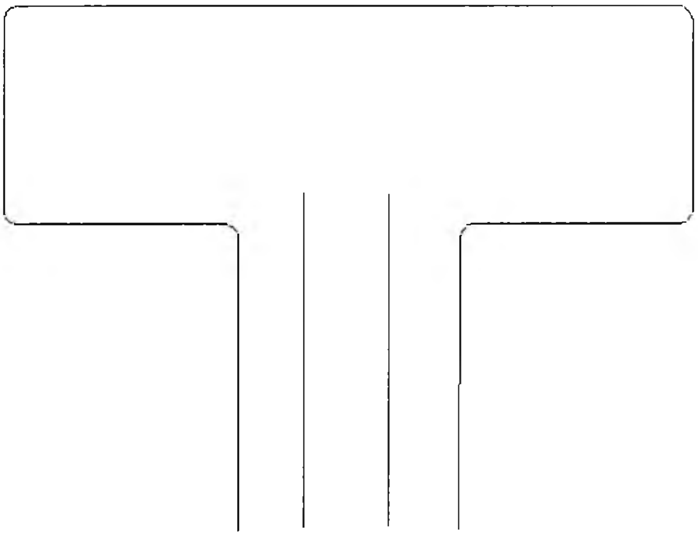


Fig.5-2 Simplified representation of the compact manifold design.

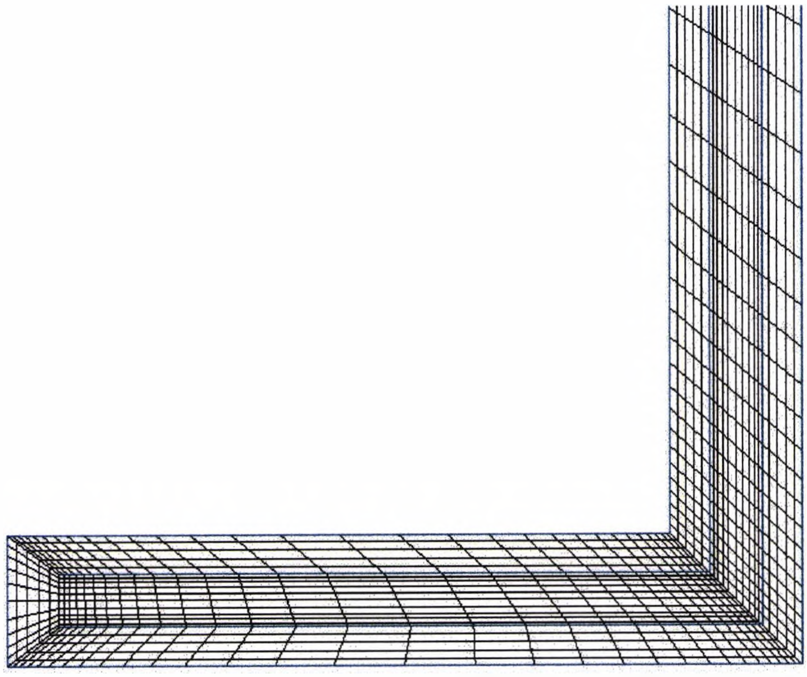


Fig.5-3 Grid used for the L shaped manifold.

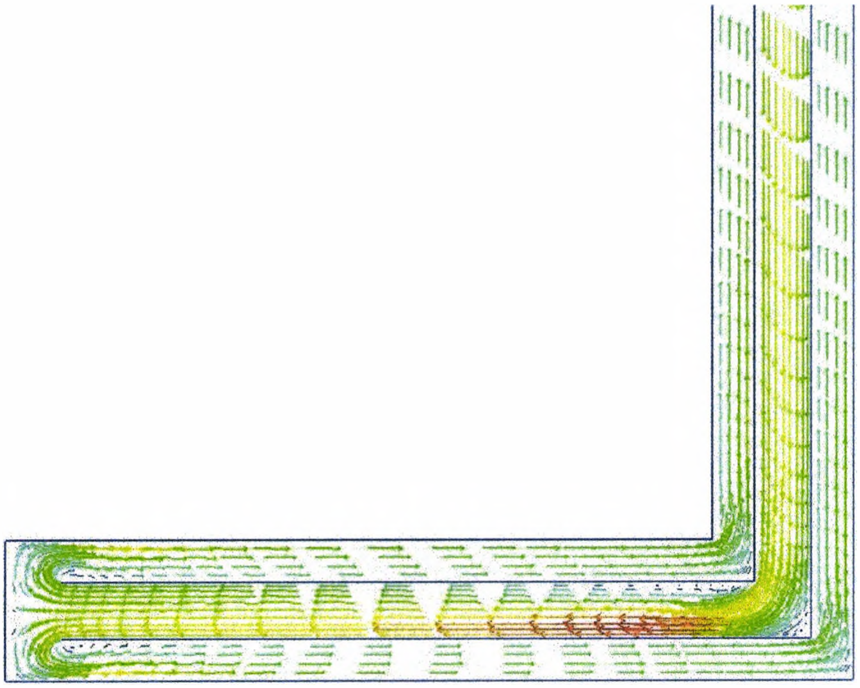


Fig.5-4 Flow pattern in the L shaped manifold at an inlet velocity of 10m/s.

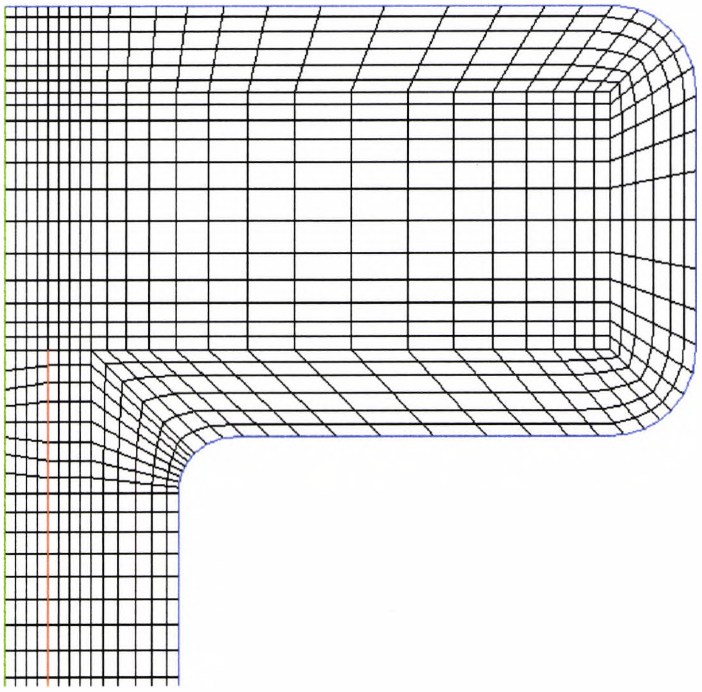


Fig.5-5 Grid used in the half section of the compact manifold design.

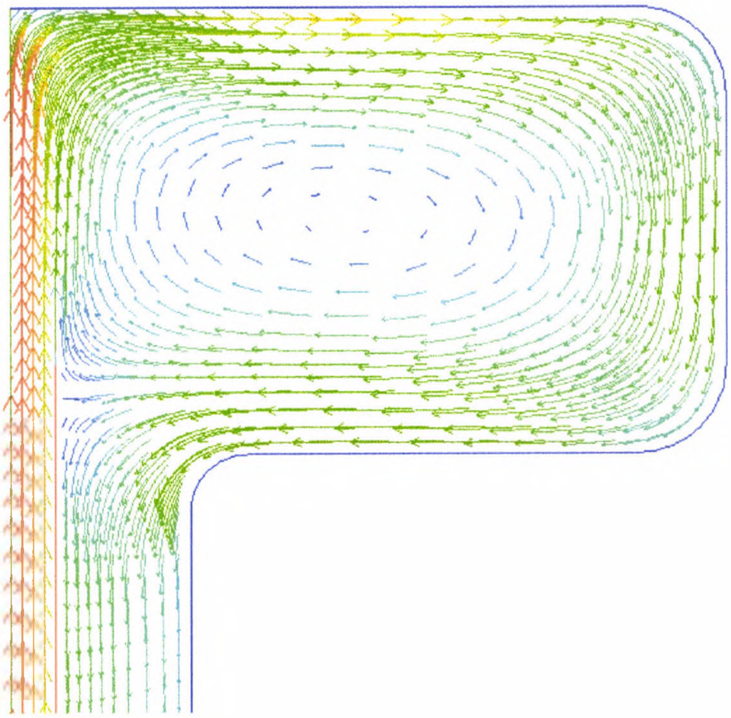


Fig.5-6 Flow pattern in the compact manifold at an inlet velocity of 10m/s.

CHAPTER-6
ELECTROCHEMICAL MODELLING

6.1- INTRODUCTION

In an effort to investigate the performance of a solid oxide fuel cell power module in a cell design, a system model has been developed building on the results of a single cell model and a stack model. These results can be coupled with a structural model to optimize the electrochemical performance and mechanical stability requirements. In addition to the mechanical and structural stability, a solid oxide fuel cell must have electrical and electrochemical performance acceptable to meet the operating requirements of specified power generation applications. The electrochemical performance of a cell depends on various factors including: cell internal resistance, material geometry, hydrogen/oxygen partial pressures, operating temperature, and rate of reaction.

The electrochemical and thermal stress models are not separable as the mechanical and electrical requirements of the fuel cell performance are interdependent. In this chapter, a mathematical model and analysis of the electrochemical performance is presented. The model is used to predict cell behavior under a variety of conditions and to investigate the effect and relative importance of various processing and operating parameters. It is also used to determine the minimum required rate of fuel flow and the number of cells in series needed in a stack to achieve a given fuel utilization percentage.

In terms of electrochemical performance, the aim of the design is to achieve high voltages (at a given current density) with low ohmic and polarisation losses to increase the overall efficiency.

6.2- GOVERNING EQUATIONS

The mathematical modeling of solid oxide fuel cell performance is typically based on formulating and solving simultaneous mass, energy, and potential balance equations. Such a model provides voltage/current density characteristics, current distribution, and temperature distribution of the cell. The potential at any given point across the cell is defined by Nernest's equation thus the name Nernest potential (*E_r*) [97].

$$E_r = E^0 + \frac{RT}{nF} \ln \left[\frac{P_{H_2} P_{O_2}{}^{1/2}}{P_{H_2O}} \right] \qquad [6\text{-}1]$$

$$E^0 = \frac{-\Delta GT}{nF} \qquad [6\text{-}2]$$

Where *R* is gas constant, *T* is temperature, η is number of equivalents, *F* is Faraday constant, ΔG is standard Gibbs free energy change, P_{H2}, P_{O2}, and P_{H2O} are partial pressures of hydrogen, oxygen and water respectively.

The resistance to current flow and the entropy change of the electrochemical reaction generate heat in the electrolyte layer. This released heat *Q* is given by:

$$Q = \frac{I}{nF}(-\Delta H_T) - EI \qquad [6\text{-}3]$$

Where ΔH is the change in enthalpy and *I* is current across the cell.

The energy balances and the heat transfer between the solid fuel cell component layers and the flowing fluids are given by the following equations.

$$m_{ia} C_{pa} (T_{ia} - T_d) - m_a C_{pa} (T_a - T_d) + A h_a (T_e - T_a) + A U (T_f - T_a) = 0 \qquad [6\text{-}4]$$

$$m_{if} C_{pf} (T_{if} - T_d) - m_f C_{pf} (T_f - T_d) + A h_f (T_e - T_f) + A U (T_a - T_f) = 0 \qquad [6\text{-}5]$$

$$Q - A h_a (T_e - T_a)_{AV} - A h_f (T_e - T_f)_{AV} = 0 \qquad [6\text{-}6]$$

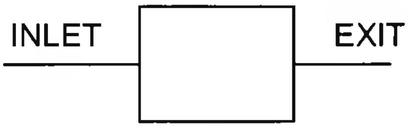
Where *m* is mass flow rate, *A* is active surface area, *U* is overall heat transfer coefficient, and C_p is specific heat. Suffixes *a* and *f* stand for air and fuel respectively.

The model is based on the combined cell configuration. It can also be adopted for use in the other cell in series configurations with a mere alteration of the input data. The cross sectional view of the combined cell design is shown in Fig.4-17.

The yittra stabilized zirconia of 180 microns thickness and 3 cm diameter electrolyte is sandwiched by the anode and cathode. The anode is made of Nickel-YSZ cermet material and has a thickness of 25 microns lying on top of the electrolyte. The cathode on the other hand, is placed beneath the YSZ electrolyte and has the same thickness as the anode. The electrodes and electrolyte are made into a washer shape geometry with the inner hole to allow a passage for the fuel. The interconnect is made into a cylindrical wall connecting the anode of one cell on to the cathode of the next in the electrical series. The cells in stack form a cylindrical geometry with the anode inside the cylinder and the cathode on the outside. The interconnect serves as a barrier between the air and fuel. Thus an airtight sealing mechanism at the interconnect electrode connection is necessary.

6.3- SOLUTION ALGORITHM

The cell geometry is divided into partitions (finite elements) along the fuel flow path for analysis. Each element is referred to as a node, which has its own inlet and exit points.



At the node inlet, the temperature is defined by the boundary conditions and the average partial pressures in the node are assumed. From this, the first estimate of Nernest potential is obtained. The energy balance equations are then solved iteratively to determine the average electrolyte temperature in the node and the temperatures of the fuel and air streams leaving the node (node exit). The electrolyte temperature is used to calculate the cell resistance and the current generated in the node.

$$I = \frac{E_r - V}{R} \qquad [6\text{-}7]$$

$$I = \eta F\left(\frac{df}{dt}\right) \qquad [6\text{-}8]$$

Where V is cell voltage and $\frac{df}{dt}$ is the rate of fuel consumption.

The amount of fuel and oxidant consumed is calculated from the current to determine the new composition of the streams. The calculated compositions are then used to calculate the partial pressures of the components at the node exit, which in turn are used to update the estimates of the average partial pressures. This iteration continues till the average partial pressures have converged.

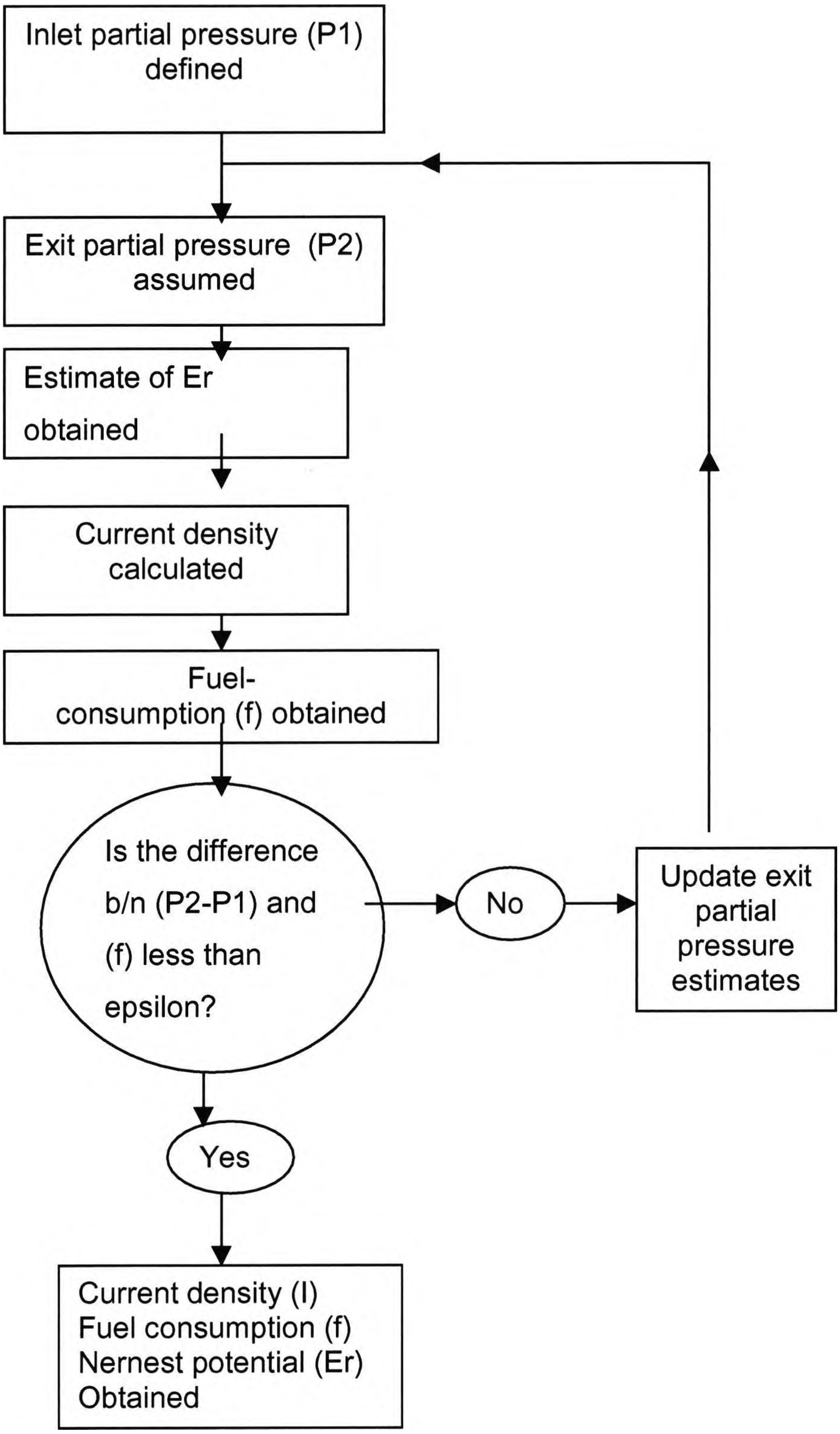


Fig.6-1 Electrochemical model algorithm

6.4- RESULTS AND DISCUSSION

To point out the effect of particular parameters on the operating conditions of a stack, a reference case is defined. The model uses input data that can be classified into three categories:

(1) Geometric data, i.e., the physical dimensions of the cell, thickness of the anode, electrolyte, cathode, and interconnect layers, flow channel dimensions, etc.;

(2) Materials data, i.e., physical properties of cell materials, such as their density, resistivity, etc.;

(3) Process data, i.e., compositions, temperatures, and pressures of the inlet fuel and oxidant streams, cell voltage, etc. The values of input parameters are given on the table below.

Input data

Electrolyte thickness, microns	180.0
Cathode thickness, microns	25.00
Anode thickness, microns	25.00
Interconnect length, cm	5.000
Anode resistivity, ohm-cm	0.001
Cathode resistivity, ohm-cm	0.013
Interconnect resistivity, ohm-cm	0.500
Electrolyte resistivity, ohm-cm	9.980
Volume fraction H_2 in fuel inlet	0.970
Inlet temperature, k	1273
Fuel inlet flow, L/h	10.00
Volume fraction of O_2 in oxidant inlet	0.210
Cell operating voltage, V	0.750

Previous work by Bossett [12] have shown that, due to the very fast reforming reaction, methane is completely converted in the first 15mm of the cell. The hydrogen partial pressure increases while water is consumed in this area. The temperature breaks down due to the strong endothermal reforming reaction, which causes the maximum Nernest potential to shift somewhat down stream. For this particular analysis, however, the maximum current density is taken as the reference point i.e., the starting edge is shifted downstream and is assumed as the fuel inlet.

For the counter-flow of fuel and air arrangement, air has its maximum temperature at the location where there is a drop in temperature due to endothermal reaction. This works towards counter balancing the negative effect a drop in temperature would have on the cell efficiency.

The primary outcome of this study is to provide overall performance curves for a solid oxide fuel cell stack in a similar manner for components such as pumps or heat exchangers. With these curves, a fuel cell could be integrated into a power system with minimal difficulty and improved accuracy. All the results were obtained from the electrochemical model (Appendix-c) by using the input data given in section 6-4.

Fig(6-2) shows the hydrogen partial pressure curve as a function of distance from the starting edge in the direction of fuel flow. The oxygen partial pressure is conveniently ignored, as the drop in oxygen concentration is insignificant considering the rate of air flow needed to heat the cell system as well as for electrochemical purposes. The hydrogen concentration is particularly important, as it is an indicator of the degree of fuel consumption and current density across the stack. The curve indicates that the hydrogen partial pressure drops off rapidly in the direction of fuel flow as it is consumed in the electrochemical reaction. The curve would show a slightly faster drop of hydrogen concentration near the inlet compared to the outlet edge, if concentration polarization across the cell was considered rigorously. The effect on the overall cell performance, however, does not differ significantly if a constant average concentration polarization is assumed instead, for the sake of simplicity.

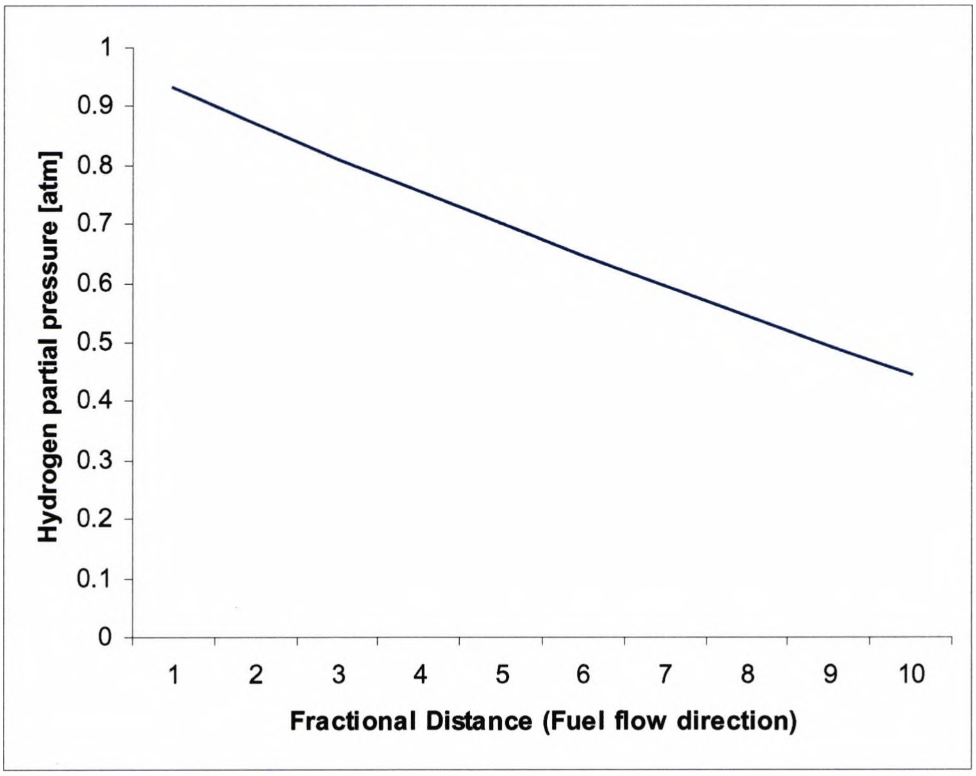


FIG.6-2 Hydrogen partial pressure distribution across the cell

The current density distribution across the cell exhibits similar curve to the hydrogen concentration. The two variables are proportional as established in equation[6-8]. The current density drops off as we go from the inlet to the outlet edges in the direction of fuel flow as shown in Fig(6-3). The variation in the direction of air flow due to oxygen concentration and temperature profile is so little that it is ignored in this analysis. The current density is expected to be slightly higher near the air outlet compared to the inlet due to higher electrolyte temperature at that location.

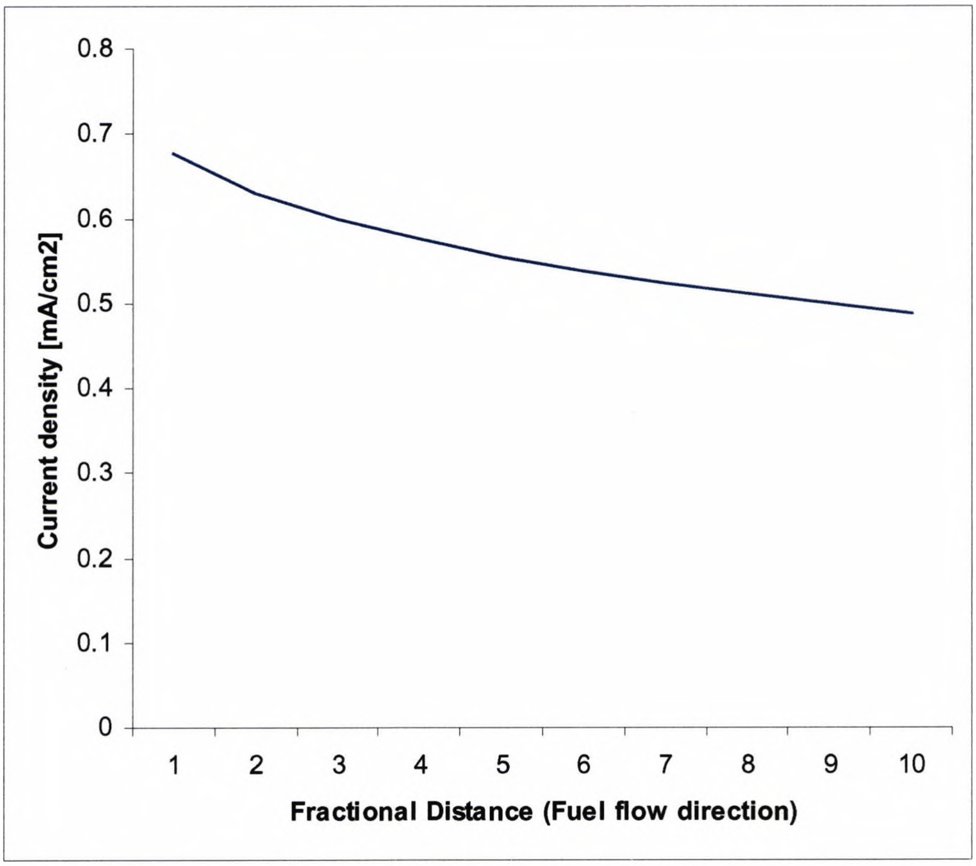


FIG.6-3 Current density distribution across the cell

The other important cell performance measuring parameter is the Nernest potential or voltage across the cell shown in Fig(6-4). According to equation[6-1], the Nernest potential is proportional to the logarithm of the partial pressures. It is high near the fuel inlet and drops off as the hydrogen in the fuel stream is replaced by water as the fuel gas flows from the inlet to the outlet edge.

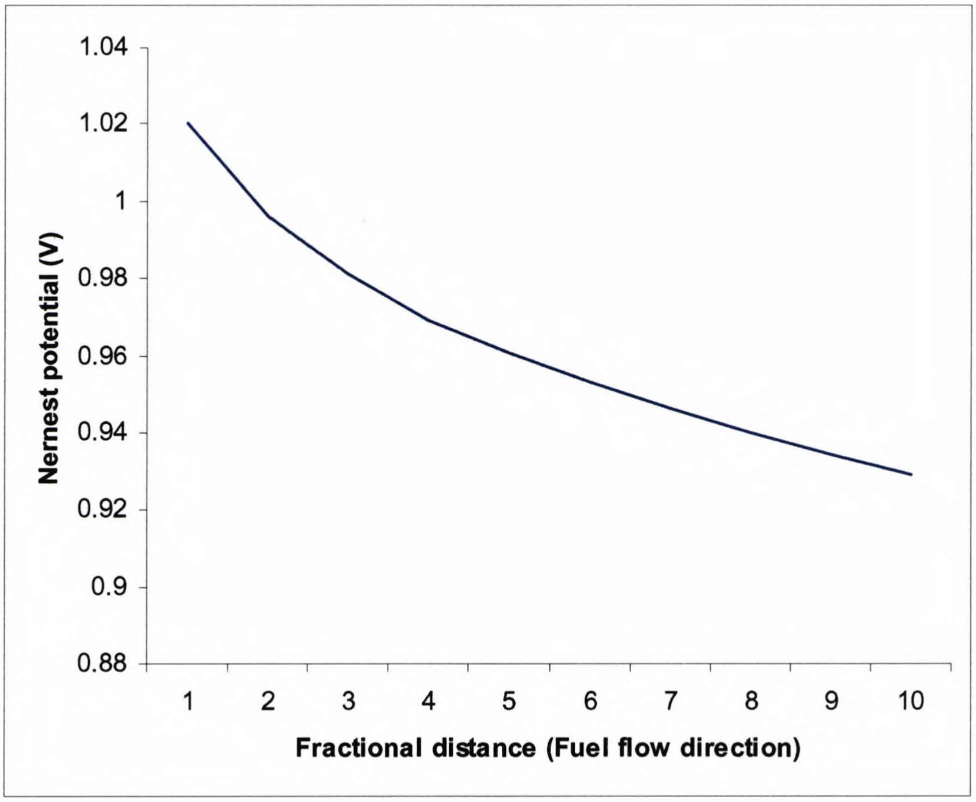


FIG.6-4 Nernest potential distribution across the cell

The electrolyte temperature across the cell layer greatly depends on the air-flow direction and current density. High current densities generate large amounts of heat and the air at the outlet of the cell has its highest temperature. Hence the maximum electrolyte temperature lies at the intersection of fuel inlet and air outlet. This point can vary depending on the type of flow employed. i.e., co-flow, counter-flow, or cross-flow. The electrolyte temperature profile is much more important in cell configurations like tubular as we have a larger surface area in a single cell. Its effect is much less significant in segmented cell in series designs. A huge temperature difference across the cell is not desirable as it causes thermal stress build up which reduces the operating life of the cell. It is therefore essential to limit the thermal stresses to an acceptable level, which might mean reducing the active surface area in the cell.

Hydrogen and oxygen rates greatly depend on the respective parameter's rates of flow. Airflow rate around the stack, as discussed in the previous chapter, is mainly dictated by the pressure drop across the geometry as well as heat transfer and electrochemical requirements. Reducing the air flow rate results in increased oxygen utilization percentage. Hydrogen utilization, on the other hand, is an important parameter with respect to the overall efficiency. The fuel flow rate is mainly dictated by the fuel utilization percentage. The rate of reaction and concentration polarization are the other factors that affect the fuel consumption. Hydrogen consumption determines the surface area in the stack or the length of cells in the series if surface area is kept constant. Cells added in series beyond the point where fuel is totally consumed are simply redundant.

The operating voltage of the cell strongly influences the power production and general performance of the fuel cell. The effect of varying the cell voltage is shown in Fig.6-5 to 6-8. The calculations are based on constant cell temperature and fuel utilization percentage. Fig(6-5) shows the effect of cell voltage on the gross power obtainable. From the figure, the optimum operating voltages at which the gross power is maximized can be determined. At high cell voltages, the gross power increases with decreasing voltage, with further reductions in cell voltage, however, the increase in cell current does not make up for the decrease in voltage, which results in lower total power generation.

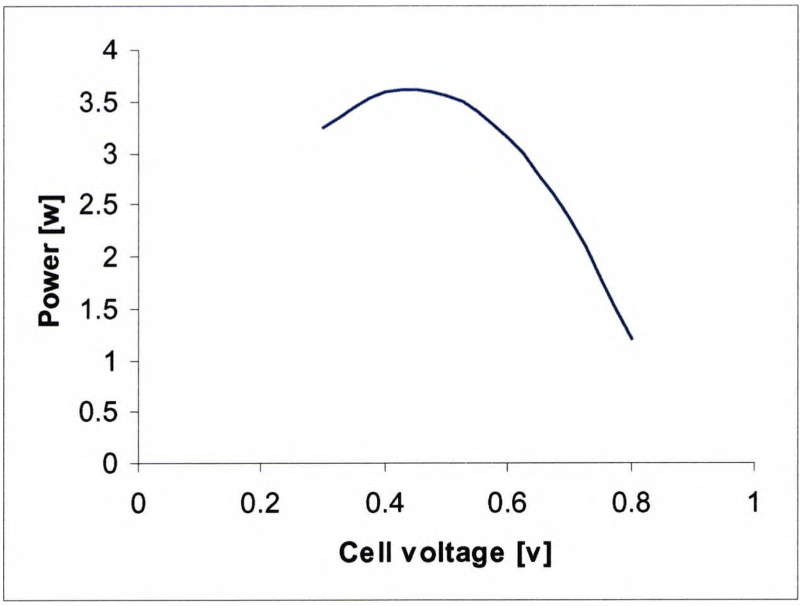


Fig. 6-5 Gross power generation as function of cell voltage

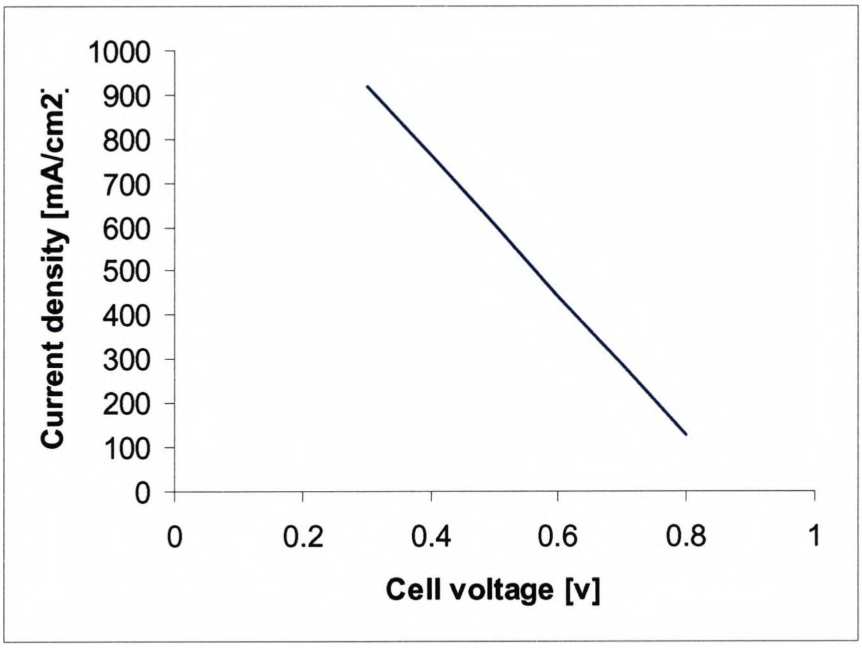


Fig. 6-6 Average current density as a function of cell voltage

The average current density decreases linearly with increasing voltage as shown in Fig(6-6). Since the fuel consumption is maintained at a constant level, the Nernest potential remains constant. The average resistance (Rav) also remains essentially constant since the cell temperature is kept constant. This, according to equation [6-7] gives the relationship a linear behavior.

The cell voltage is adjusted to the required level for a maximum power output and efficiency by choosing an appropriate rate of fuel flow at a constant fuel utilization level. Since fuel consumption is linearly proportional with the current density and the current density has a linear relationship with the cell voltage in turn, fuel consumption is related to the voltage in a linear manner as shown in Fig(6-7). The required fuel flow rate increases with decreasing cell voltage.

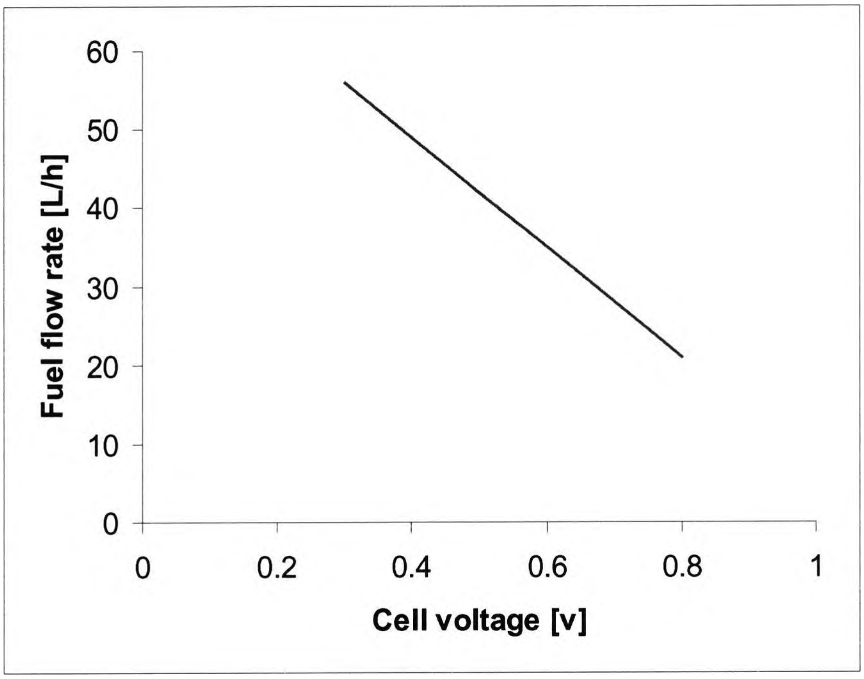


Fig. 6-7 Fuel flow rate as a function of cell voltage

As the fuel flow rate required to maintain a given fuel utilization percentage at a constant temperature decreases with an increase in cell voltage, the fuel efficiency increases with an increase in voltage a shown in Fig(6-8).

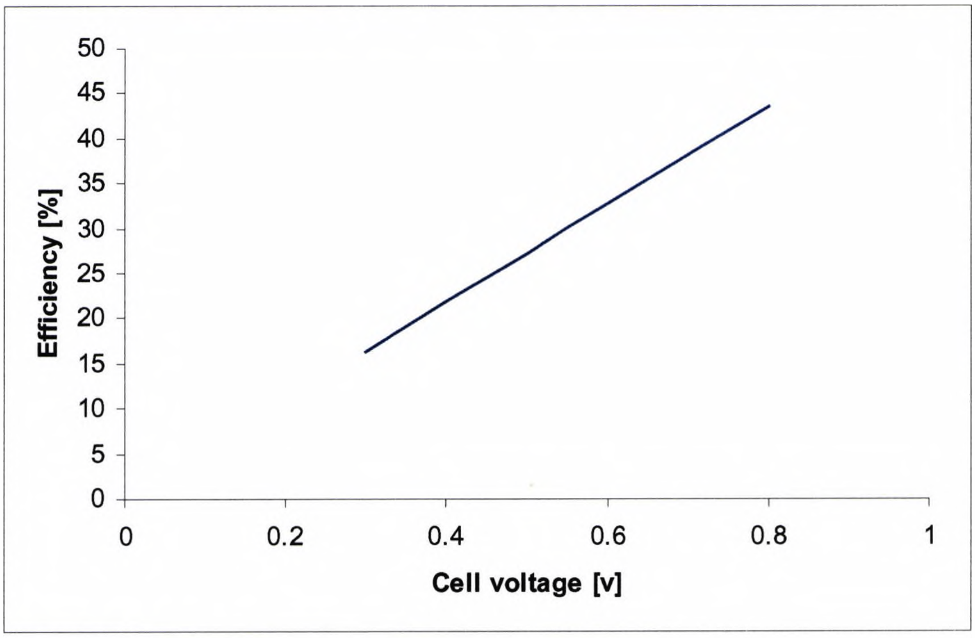


Fig.6-8 Efficiency as a function of cell voltage

The model predictions are used to determine the cell geometry, air and fuel flow rates and to evaluate the effect of varying design and operating parameters on the overall cell performance. The model results are by no means a replacement for experimental data. They, however, reduce the need for extensive experimentation before knowledge on performance is obtained. In other words, this is in line with the philosophy of achieving a quality product at a lower cost by reducing down stream design changes.

CHAPTER-7
MECHANICAL RELIABILITY

7-1 INTRODUCTION

This chapter is concerned with understanding the mechanical behaviour of the planar solid oxide fuel cells. This includes analysing the stress generating mechanisms and calculating the stresses across the cell geometry in order to predict the modes of mechanical failure. Calculating these stresses requires data about the mechanical properties of the cell components, which is scarce.

The stress distribution influences not only the mechanical reliability of the cells but also electrochemical performance. A crack in the electrolyte, for example, can cause leakage of the fluids from one reaction site to the other resulting in losses. Or, de-lamination across the interface between electrolyte and electrodes would lead to performance degradation. The stress distribution across the cell dictates the failure mode. Evans and Hutchinson [49] have shown that a thin film sintered on a thicker substrate fails in the mode of delamination if under compressive stress. A film under tensile stress fails in the manner that initial cracks around the edge propagate across the interface or towards the depth into the substrate depending on the bonding strength between the two layers, electrolyte and electrodes in the case of SOFCs.

There are many mechanisms responsible for generating stresses in the planar SOFC. These include:

1- residual stress due to thermal expansion coefficient mismatch between the cell components,
2- Temperature gradient across the cell,
3- Variation in oxygen partial pressure mainly affecting the mechanical properties of the cathode,
4- Mechanically applied loads.

With in a single cell, residual stress due to thermal expansion mismatch between the different layers is the most dominant mechanism for stress generation in planar SOFCs. This study will be confined in the calculation of the residual stresses using experimental and Finite Element Analysis.

7-2 ELASTIC PROPERTIES OF CELL COMPONENTS

Ceramic materials have a large scatter in mechanical properties strongly dependent on the manufacturing procedure. This generates the need to characterise the material properties in relation to their manufacturing history. Sintering temperature greatly affects the porosity which in turn is the most important factor determining the elastic moduli of ceramics. Many equations have been developed to try and predict the influence of porosity on the elastic properties of ceramics using both theoretical and empirical techniques. Elastic properties of materials are also known to depend on temperature. Lowrie [89] measured the variation of young's modulus with temperature of sheets of 8YSZ over a temperature range 20 – 950^{o}c.

Young's modulus and thermal expansion coefficient are the most important properties affecting the residual stress build up. There are different mechanical testing methods employed to characterise these properties. The coefficient of thermal expansion can be measured from a simple arrangement using delatometer calibrated against a sapphire standard specimen. A tensile test used to determine the elastic modulus of metals is not applied for ceramics as these materials exhibit different properties in tension and compression, and since it is difficult to hold a thin ceramic specimen in a tensile testing machine. Ring-on-Ring bi-axial test is commonly used as it also reflects the loading conditions of SOFC in this project.

7-2-1 RING-ON-RING EXPERIMENTAL ARRANGEMENT

Circular disks in bending have been extensively used for strength tests of brittle materials. The disks are supported on a continuous circular ring and are loaded by a concentric ring of smaller diameter.

The stress distribution across the thin circular plate under the ring-on-ring test is such that the maximum stress occurs inside the inner loading ring. Both the tangential and radial stresses within the inner ring are equal as shown on Fig.7-1.

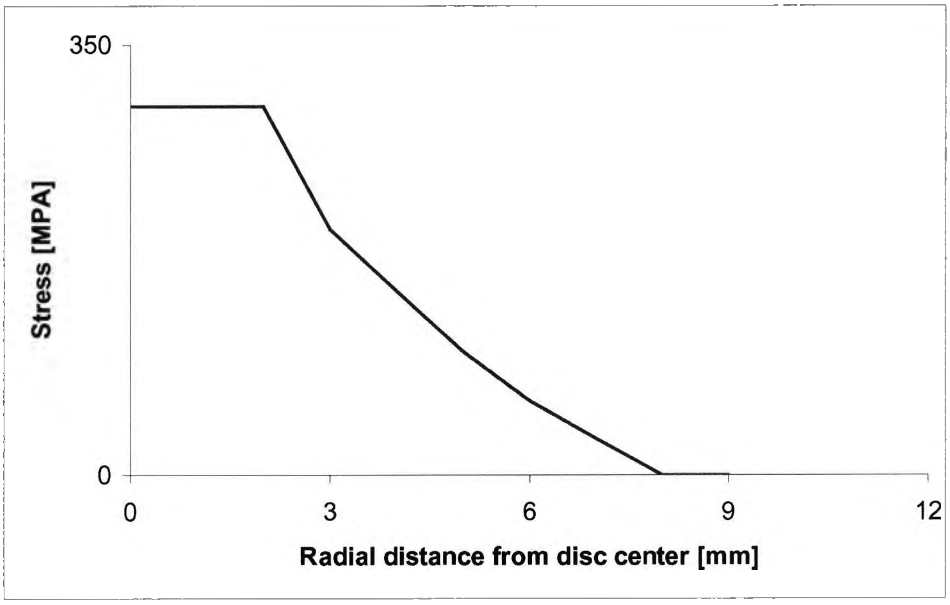


Fig.7-1 Stress distribution in a ring-on-ring test

The equibiaxial uniform stress area is the area of interest in determining the Young's modulus of the disk specimen. The ring-on-ring test has been extensively used for strength measurements on ceramic materials and has been standardised (e.g. German standard DIN 52292).

This however is only applicable for a bulk specimen. Hence only the elastic modulus of the bulk YSZ can be characterised directly.

The experiment was carried out at room temperature. For high temperature tests, a rig made of high temperature material like silicon nitride, Alumina or any other material that would be stable at cell working temperature is required. This, however, proved to be expensive, which goes beyond the budget allocated for the project.

The test rig for the room temperature strength tests was composed of a supporting ring of radius 19mm made of steel and a round ended tube as a loading ring of radius 4.75mm, which is mounted to the load cell of 200N capacity. Deflection was measured using externally mounted displacement transducer. Load-deflection data was then recorded on to a *Mac Lab* data acquisition system.

The properties of the electrodes, which are coated using screen-printing or plasma spraying, can not be measured directly from the ring-on-ring experimental arrangement. Properties of a bulk anode or cathode are not representative for the coating properties either. This necessitates for a technique to measure the properties of coats. An indirect measurement technique has been employed in the past.

7-2-2 A METHOD FOR EVALUATING THE ELASTIC PROPERTIES OF COATINGS

Thin hard coatings are today successfully utilised to improve the performance of a wide range of components in a vast number of engineering applications. Some of the important applications other than SOFCs, include the use of thermal coatings in gas turbine blades. If prediction of the coating performance is to be made, coating material properties such as Young's modulus must be known.

A method to evaluate the coating properties has been proposed by Hollman et al [69], which uses a composite tensile specimen consisting of a core alloy of well-characterised elastic properties on to which the coating is deposited. The overall elastic modulus of the specimen is determined and this can then be deconvoluted to obtain the properties of the coating. The method has the advantage that the coatings are evaluated for the same microstructural conditions as they will be used under, i.e. having the same porosity levels and microstructure.

Testing and evaluation of thin hard coatings is not, however, easily performed. Several experimental difficulties arise from, among other things, the fact that the coating is extremely thin as compared to the substrate thickness. Therefore, the substrate usually influences the raw test data greatly, which makes it hard to extract the coating's influence on the overall performance.

In this study, a biaxial measurement technique is employed as it is suitable for ceramic materials and represents the loading conditions in the planar solid oxide fuel cells. Benabdi and Roche [13] have established the relationship between the combined Young's modulus of the two layers with the individual components of the composite (equation 7-1). The Young's modulus of the bulk substrate and the composite are measured from the ring-on-ring set up and that of coating can be derived from the relationship.

$$(EI)_{eq} = E_c I_c + E_s I_s + \frac{E_c S_c E_s S_s \left(\frac{h_c}{2} + \frac{h_s}{2} \right)^2}{E_c S_c + E_s S_s} \quad \text{.......} [7-1]$$

Where, *E* is young's modulus, *I* = moment of inertia, *h* = thickness, *S* = *bh, where b*= width and subscripts *eq*, *c* and *s* stand for the equivalent, the coating and the substrate respectively.

7.2.3- MEASUREMENTS USING LOAD DEFLECTION CURVES

Young's modulus of ceramic materials is known to decrease significantly with increase in temperature. In this study, measurements are confined to room temperature. The Young's modulus is calculated from the load deflection curve by applying thin plate theory. The deflection at the centre of the thin circular plate is related to the Young's modulus by the theory of plates and shells as:

$$M_r = -D\left(\frac{d^2\omega}{dr^2} + \frac{vd\omega}{rdr} \right) \quad \text{.......} [7-2]$$

$$M_t = -D\left(\frac{1}{r}\frac{d\omega}{dr} + v\frac{d^2\omega}{dr^2} \right) \quad \text{.......} [7-3]$$

Where, ω is the deflection *dω/dr* is the slope of the curve and *D* is defined as the flexural rigidity of the plate given by:

$$D = \frac{Eh^3}{12(1-v^2)} \quad \text{.......} [7-4]$$

Where, *E* is Young's modulus, *h* is plate thickness and υ is Poison's ratio. From the above equations, the Young's modulus of the plate was calculated by substituting the measured values of load and deflection. Fig.7-2 shows the calculated young's modulus for each specimen.

Specimen	**Young's modulus from R-o-R test [GPa] (mean)**
YSZ	190
Anode – YSZ	153.3
Cathode – YSZ	160.6

Fig.7-2 Young's modulus of the YSZ and bi-layers from the ring-on-ring test.

The equivalent Young's modulus of the bi-layers were substituted into equation [7-1] to calculate the values for the corresponding coatings. The elastic modulus for the anode (NiO-YSZ) was found to be 55 GPa and that of the cathode (LSM) was 35 GPa. This values were then compared with theoretical predictions made as a function of porosity by Mackenzie [93] and Budiansky [26].

Material	Young's modulus of fully dense bulk material (E_o) [GPa]	Coefficient of thermal expansion [cm/cm k]	Poisson's ratio
YSZ	200	1.08E-5	0.3
NiO-YSZ	231	12.8E-5	0.3
LSM	240	1.2E-5	0.3

Fig. 7-3 Room temperature properties of fuel cell materials taken from Minh [97]

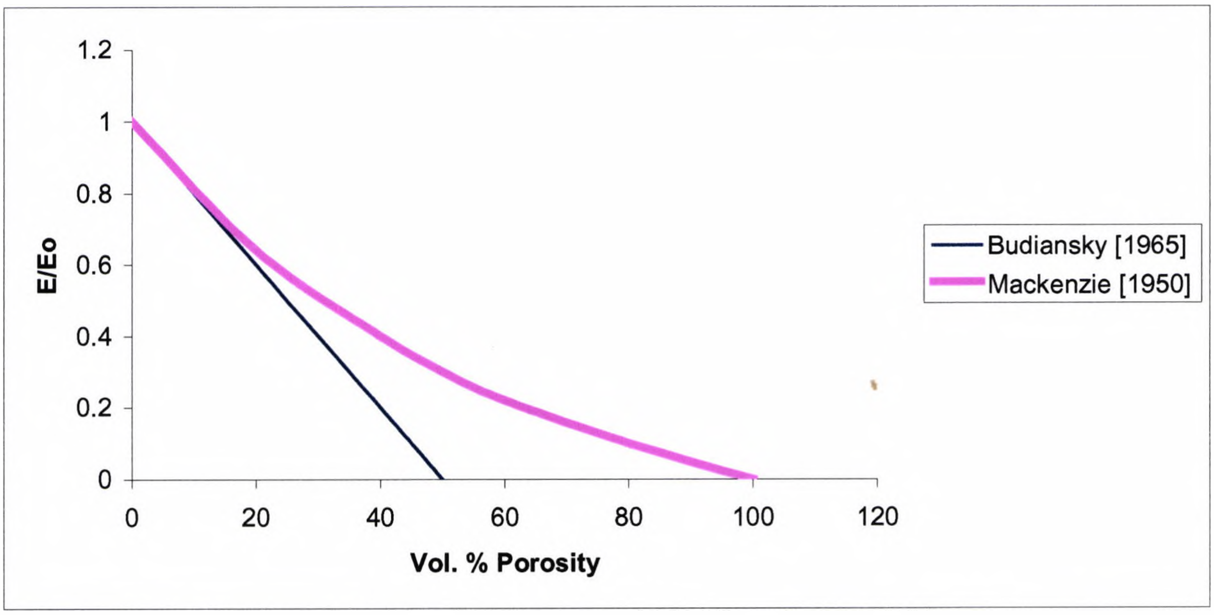


Fig.7-4 Predicted Young's modulus as a function of porosity

The porosity of the anode and cathode coatings was estimated from the density measurements of the bi-layers. The anode and cathode were found to have a porosity of 36% and 41% respectively. Using this porosity values and their properties at full density (Fig.7-3), Mackenzie's predictions give a value of 108.5 GPa for the anode and 91.2 GPa for the cathode, which greatly overestimates the Young's modulus. Budiansk's predictions were closer to the calculated values at a 64.7 GPa for the anode and 43.2GPa for the cathode.

7.3- RESIDUAL STRESS

An understanding of the significance of the mechanical stresses with in the fuel cell stack is required to design a fuel cell which will not exhibit poor performance or reduced life time.

Residual stresses generated during sintering of ceramic-based fuel cell components can lead to cracking or delamination. Predominantly these stresses are caused by thermal expansion coefficient mismatch between cell components.

The stringent electrochemical requirements for fuel cell materials limit the choice of materials and the possibility of well matched thermal expansion coefficients.

The most common method of manufacturing planar self-supported electrode/electrolyte structures is to deposit electrodes, using screen-printing or plasma spraying, on to a pre-sintered electrolyte and then sinter the electrodes. Up on cooling, from a sintering temperature to a room temperature, the layer with a higher thermal expansion coefficient (CTE) tends to shrink more than the layer with lesser CTE. The shrinkage in the plane of the layer with higher CTE is restrained by contact with the other layer generating stresses.

The stresses, which are induced by the differential thermal expansions, can be determined by considering a simplified bi-layer stack. For equilibrium, the stresses in layer one, σ_1, is given by:

$$\sigma_1 = \frac{\kappa E_2 h_2^{\,3}}{6h_1(h_1 + h_2)(1 - \nu_2)} \qquad [7-5]$$

Where, h = thickness, E = young's modulus, υ = Poisson's ratio, κ = radius of curvature of the bi-layer and subscripts 1 and 2 represent layers 1 and 2 respectively.

7.3.1- MEASUREMENT OF RESIDUAL STRESSES

The residual stresses at room temperature were estimated from curvature of the laminates and the elastic constants of the individual layers. The out-of-plane distortion of the laminated discs was measured using a ' Talysurf ' surface profiler. Two scans in orthogonal directions were made on three specimens of each bi-layer (i.e. Anode-YSZ and Cathode-YSZ). A typical result is shown in

Fig.7-5. Accurate measurement of residual stress of a tri-layer composite is not possible due to the fact that one layer can counter balance the effect of the other layer. A typical example is when the tri-layer is made of a substrate and a coating of the same material and geometry on opposite faces. Despite the existence of a residual stress, there appears to be no curvature as one layer balances out the effect of the other.

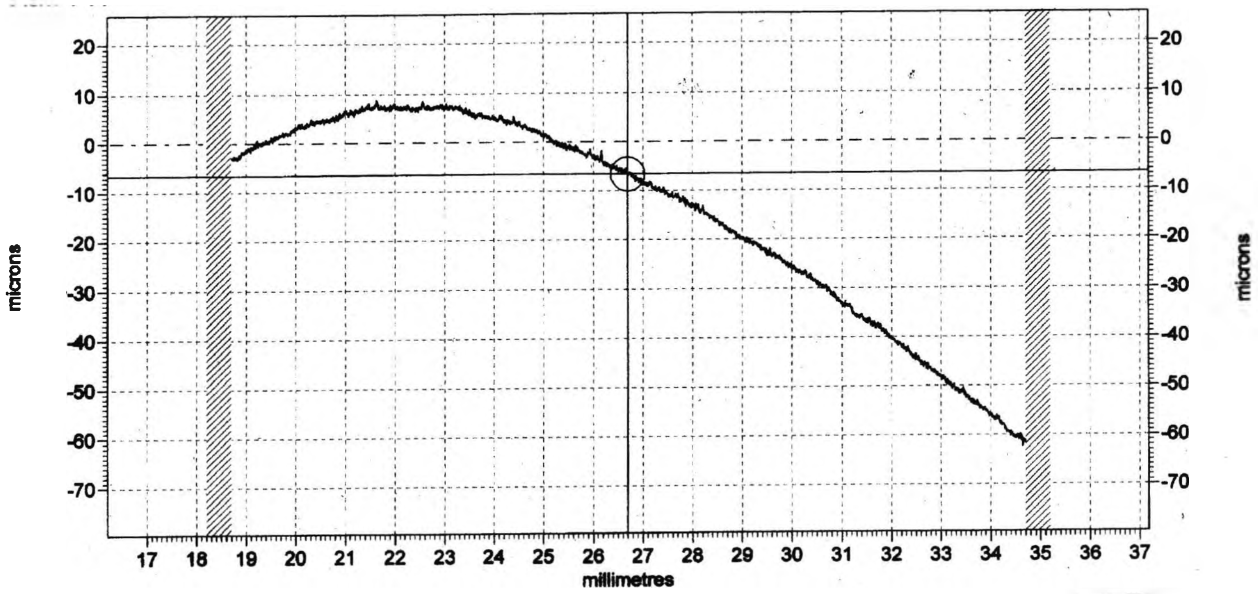


Fig.7-5 A raw surface profile of anode + electrolyte bi-layer

The FE prediction of stress on the cathode (Fig.7-9) shows a much lower value compared to the anode due to lower CTE and lower Young's modulus. The analysis, thus, concentrates on the anode. The profile in Fig.7-5 was converted into a curve fit to obtain a radius of curvature of 2332±10 mm. This was substituted in equation [7-5] along with the elastic properties and the resulting residual stress distribution at room temperature was found to be 50.64MPa. This, compared to the FE results calculated from the thermal expansion mismatch up on cooling from the sintering temperature of 1300°c to room temperature was found to be lower. The FE results predicted tensile stress of 78 MPa on the anode layer (Fig 7-7). This suggests that some stress relief had occurred during cooling.

In fact, good agreement between the two was obtained if it was assumed that the specimens were stress free at temperatures above 900°c, for which condition the FE results predicted a residual stress of 52MPa (Fig.7-8). This can happen if the stress on cooling from 1300°c to 900°c had been relieved by plastic deformation (creep). Characterisation of the creep behaviour of materials can verify the conclusion. This, however, is beyond the scope of the present work. A scan electron microscope image of the anode, Fig.7-6, shows micro-cracks occurring in the plane of the anode which are responsible in relieving some of the stresses. The residual stress on the tri-layer (anode – electrolyte – cathode) is then predicted from the FE analysis at a stress free temperature of 900°c as shown in Fig.7-10.

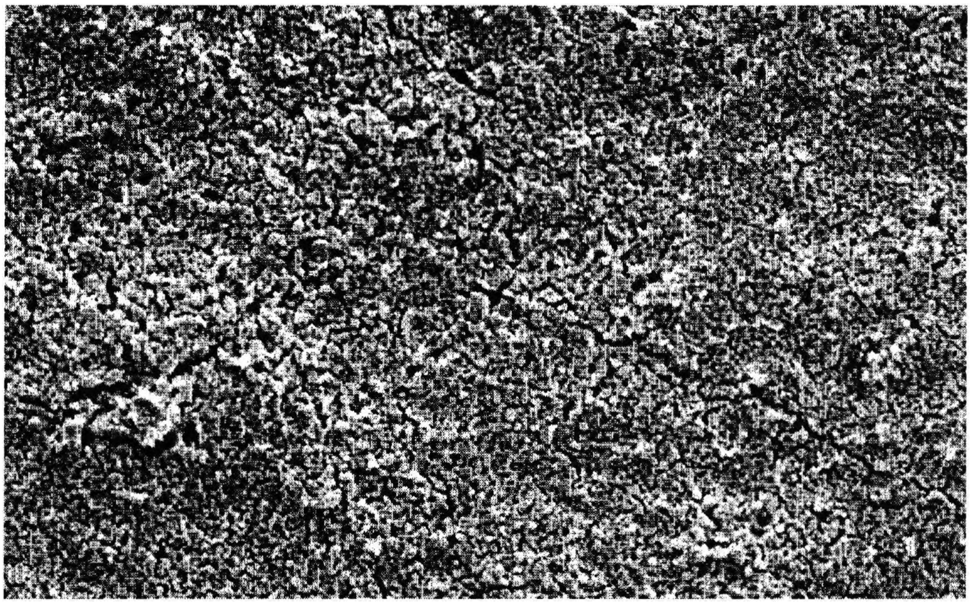


Fig.7-6 SEM image showing the surface of anode layer. (X500-mag)

All FE analysis was performed using the Finite Element code ABAQUS. The quarter of actual geometry of the proposed conceptual design was modelled due to symmetry using solid continuum elements (C3D8). Symmetry boundary conditions were used.

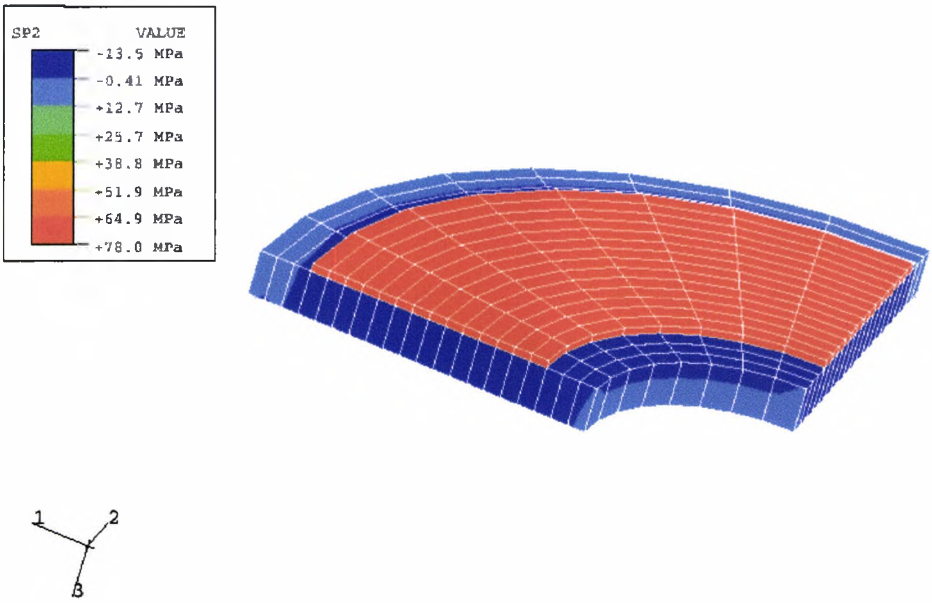


Fig.7-7 The largest principal stress distribution on the anode-ysz bi-layer from a stress free temperature of 1300°c

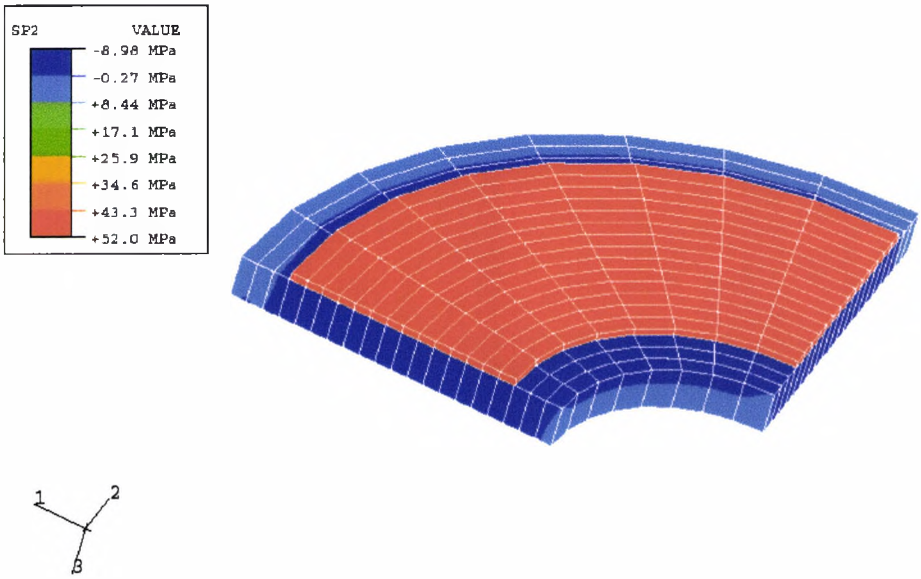


Fig.7-8 The largest principal stress distribution on the anode-ysz bi-layer from a stress free temperature of 900°c

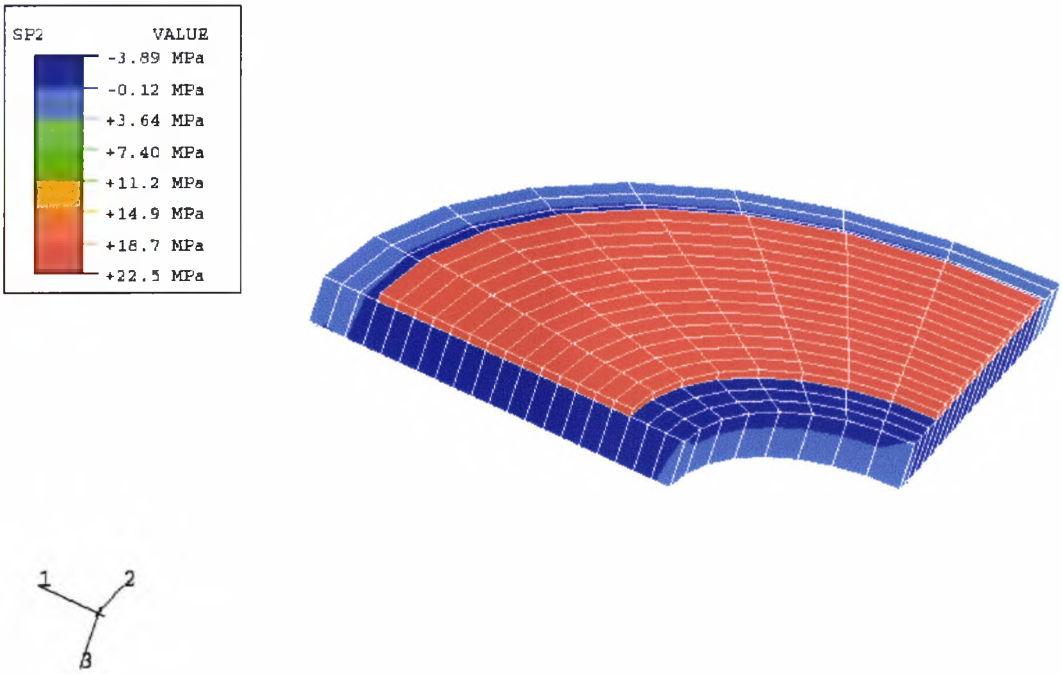


Fig.7-9 The largest principal stress distribution on the cathode-ysz bi-layer from a stress free temperature of 900°c

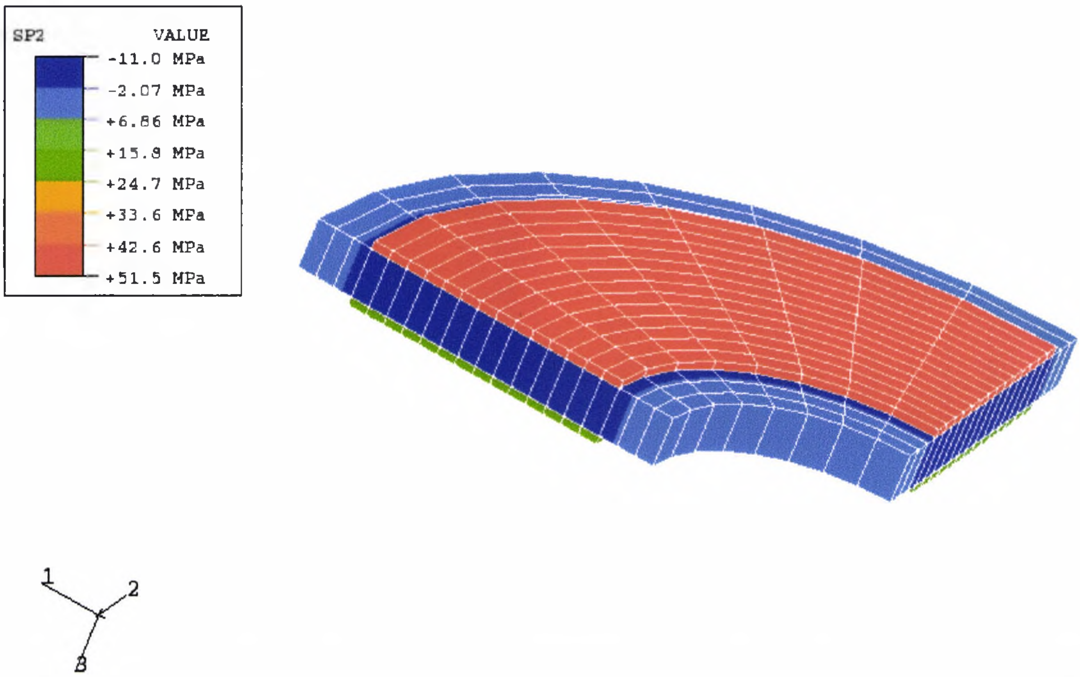


Fig.7-10 The largest principal stress distribution on the cathode-ysz-anode tri-layer from a stress free temperature of 900°c

CHAPTER-8

CELL COMPONENT FABRICATION

8.1- INTRODUCTION

The first lesson that the design-led philosophy of Taguchi gives is to push as much information back to the designer from the downstream life of the product. At the very least, it requires breaking down the barriers between the design and manufacturing functions, which are traditionally treated separately.

The purpose of the fabrication experiments is to achieve knowledge on the manufacturability of the cell components in order to decide the geometry and reduce downstream design changes. Reducing variability to build quality into the product at the design stage is the essence of Robust Engineering.

This chapter is concerned with running statistically designed experiments, interpreting the data and establishing the optimum product and process design. The robust engineering approach to product design and the Taguchi type experimentation was explored in chapter-3. It was established that an *ad hoc* experimentation of one variable change at a time was neither necessary nor cost-effective. Instead, statistical design of experiments is adopted. This means, making many design changes at once and conducting several tests and evaluations before decisions are taken on what the next step in the development process should be.

In this experiment, several variables or factors are identified; each of them is to be tested on different values or levels. A quality function is also calculated as an indicator of quality improvement or even quality loss.

The experiments were conducted at the City University workshop based on constant information-exchange with Burnstone Ceramics Ltd. Their prior experience was put into use to avoid unnecessary factor levels, which in turn reduces the degrees of freedom within the experiment.

Burnstone's help was particularly useful in choosing the factor levels. One of the most important procedures that have to be followed prior to experimentation is the proper selection of factor levels. Careful consideration of the experimental range for each factor and of the interrelationship between factors can help an appropriate choice of levels. It must not include any range which, from prior experience, is known to be unusual or worse than the others in terms of cost, acceptable yield, etc. This eliminates the possibility of failed trials or useless information.

8.2- BRIEF DESCRIPTION OF COMPACTION EXPERIMENTS

Several fabrication techniques, all based on the press sintering approach, have been attempted in order to come up with a feasible and cost effective manufacturing process. Some of the procedures followed and their short comings are listed below.

8.2.1- THE CONNICAL CONFIGURATION

Experimentation was first being carried out to fabricate components for the conical cell-in-series configuration. To form a conical green compact of yittra stabilised zirconia; a brass plate was forged into a conical shape on the surface of which the powder can be pre-formed. Brass cones of 10° half angle were prepared. The choice of the cone angle was dictated by powder compaction requirements. Larger cone angles were found to be not suitable to contain the compacted powder. Press sintering technique involves pressing the powder into a desired shape by applying a measured compaction force and then sintering to temperatures up to 1500°c for about 12 – 16 hours. Due to the obvious stability problem with brass material at such elevated temperatures, straight sintering in the furnace was not a possibility. Instead a two stage sintering process was adopted. First, the pre-formed powder supported by the brass cone was sintered in the furnace at a temperature of 700°c for eight hours. This stage is termed as pre-sintering. After the pre-sintering stage, the brass support was removed and the green compact, with no support, was put in the furnace for full sintering to a temperature of 1500°c for 12 hours. Removing the kiln furniture (brass cone) at the interval between the two sintering stages, however, caused a crack to the green-compact, which was later propagated during the full sintering. The cones were also found to shrink at a magnitude of 20% during sintering.

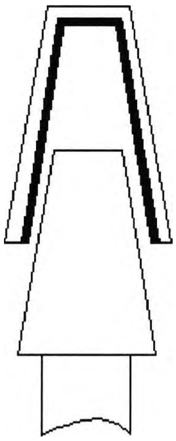


Fig.8-1 Compaction using a brass cone and a steel tool.

Two constraints were identified at this stage. The requirement for a kiln furniture that is chemically inert which will remain stable at the sintering temperature of 1500°c and the need of a mechanical support to prevent the inward shrinkage of the conical electrolyte during sintering. One suitable material for this was, a high-grade alumina which is difficult to machine. A special rigidizing cement, which was developed by Burnstone Ceramics, was used. Conical holes were drilled on the alumina board on which surface the YSZ powder was formed. The surface was first coated with cement to improve stiffness and surface finish. After forming the powder on the surface and applying a compaction force of 2 – 3 kN, it was put in the furnace for full straight sintering at 1500°c for 12 hours. To balance the inward shrinkage, a conical male part was machined to sandwich the compacted powder between the male and female parts during sintering. This greatly improved the zirconia cones produced but lacked uniformity on the thickness as the pre-forming on the conical surface was done manually. The alumina kiln furniture could only be used for one or two fabrication runs, beyond which it deteriorates and needs replacing. This proved prohibitively expensive and as a result, the conical configuration was abandoned.

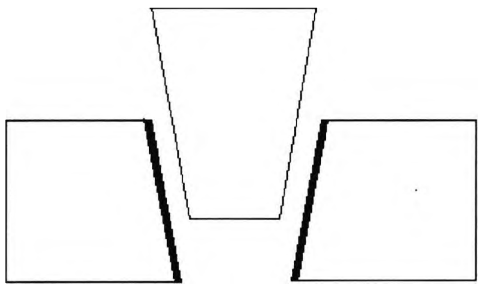


Fig.8-2 Direct compaction into male & female alumna material.

8.2.2- PLANAR CONFIGURATION

Having identified the manufacturing constraints with sintering the zirconia electrolyte, the DFD process was re-started in an effort to generate a cost effective manufacturing route that would overcome the existing constraints. Manufacturing experiments were conducted, by focussing on the cost associated with fabrication; to produce the critical washer shaped planar electrolyte (Fig.4-16). Cement rigidized alumina paper was used as a kiln furniture. A sheet of polythene material was used as a sacrificial substrate, which acts as a releasing agent that disappears during sintering. This new manufacturing route provides a cheaper way of fabricating the critical electrolyte component of the solid oxide fuel cell and there is no limitation on the geometry as in the conical configuration. Full details of the new fabrication route are not presented in this thesis.

The key design feature is the kiln furniture, which can constrain the direction of shrinkage and provide mechanical support during sintering. The conceptual design, based on the washer shaped planar electrolyte (Fig.4-16), which is an outcome of a brain storming session focused in reducing the cost, provides a cheaper fabrication route that will go a long way in reducing the cost of the over all SOFC plant. This configuration was taken to the optimisation process (chapter-9) to determine the optimum operating parameters in the cell design. The Taguchi experimental plan to study the combination of factor levels that would give the best electrolyte performance is based on this particular configuration.

8.3- DESIGN VARIABLES (FACTORS)

Identifying the factors that may bring about a difference on the product's behaviour and/or performance is the first step of a statistically designed experiment. At this stage, all the factors including qualitative i.e. those, where there is no numerical hierarchy to separate the levels and the quantitative, that are measurable on some sort of scale, are listed. The following is a list of all the variables that affect the performance and cost of a zirconia (yittra stabilised) cones to be used as an electrolyte.

1- Fabrication technique
2- Cell geometry
3- Powder grade – a coarse and fine grade powders.
4- Sintering technique – two stage sintering and straight sintering.
5- Compaction force – force used to pre-form the powder into the conical shape.
6- Sintering temperature
7- Sintering time.

The cost of fabrication of cell components is the stumbling block in the commercialisation process of solid oxide fuel cells. EVD technique is particularly costly. Hence in this experiment, press sintering is the only fabrication technique employed for the self supporting electrolyte.

Having determined the factors, which are to be kept fixed through out the experimentation, the five remaining factors were given two values each. These values are termed *levels* and are given the symbols of - & + as shown on the table below.

FACTOR	LEVEL1 (-)	LEVEL2 (+)
A- Powder grade	Coarse	Fine
B- Compaction force	2 KN	5 KN
C- Sintering temperature	$1400^{o}c$	$1600^{o}c$
D- Sintering time	12 hrs	16 hrs
E- Cooling rate	Furnace cooling	Air cooling

FIG. 8-3 Level- values of the experimental factors.

8.4- QUALITY FUNCTION (RESPONSE)

Quality function sometimes referred to as quality characteristic is defined as the yardstick where by the performance of the engineering system is characterised by a measurement of some aspect of function. Before one can measure the quality function, it is imperative to establish the intended functions of the product. The mechanical, electrical and other requirements of the yittra-stabilised zirconia material for use as an electrolyte were explored in chapter-2. The following is a list of some of the design functions or deployed requirements.

1- Adequate mechanical strength,
2- Density approaching theoretical value (negligible porosity),
3- Thickness of around 200 microns or less,
4- Wall surface finish,
5- Chemical stability,
6- Cost of fabrication.

The purpose of this is to study the effect of changes in the factor levels on the above functions. The design functions, however, have degrees of weight attached to them. i.e. not all functions are equally important for the overall quality of the product. A relative weight factor is assigned to each of the above functions according to their importance in affecting the cell performance.

Design functions	Weight factors (%)
1- Porosity (P_i)	40
2- Wall thickness (T_i)	30
3- Mechanical strength (S_i)	20
4- Cost (C_i)	10

FIG. 8-4 Weighting factors

This is not to mean that cost is least important. Since the fabrication technique and the material are fixed, the only variation in cost comes from the powder grade, which is not significant. Data from the design experiment are used to analyse the mean response. In this experiment, we do not have a simply measured quality function as a response. Instead, we have a combination of different functions with different importance ratings. The quality function can then be calculated as:

$$QF = 40Pi + 30Ti + 20Si + 10Ci$$

Where the coefficients represent the assigned values of weighting factors and the corresponding letters represent the index of the measured response values. Having assigned the weights, the relative indexing of each of the factors must be established. This index is an indicator of how the factors approach the desired values to contribute towards a better quality.

(1) Porosity

It has been established in chapter 2 that, the electrolyte must have a density approaching the theoretical value in order to prevent gases from cross-leakage. In other words, a zero porosity is ideal scenario towards achieving the quality target.

The most important aspect in the fabrication of the electrolyte is the production of a fully dense layer. In the particulate approach (i.e. the press sintering technique), the densification of powder at elevated temperatures is dependent on material and processing factors such as powder characteristics, processing conditions and particle packing. Ideally, a fully dense, thin electrolyte is required. Achieving that, however, remains a challenge. Recently, further advancements have been made to powder synthesis and processing of ZrO_2 materials. YSZ powders have been formed into a green body and fired to 95% theoretical density in air at 1125^{o}c. A 70% theoretical density (or 30% porosity) is not good enough as an electrolyte as it allows gas cross leakage and degrades the cell performance significantly. Hence the 30% porosity is given a minimum value (0 points) and the fully dense (or zero porosity) is given the maximum value (40 points) in the index scale (Fig.7-5). The values in the middle are assumed to correspond with the index in a linear manner.

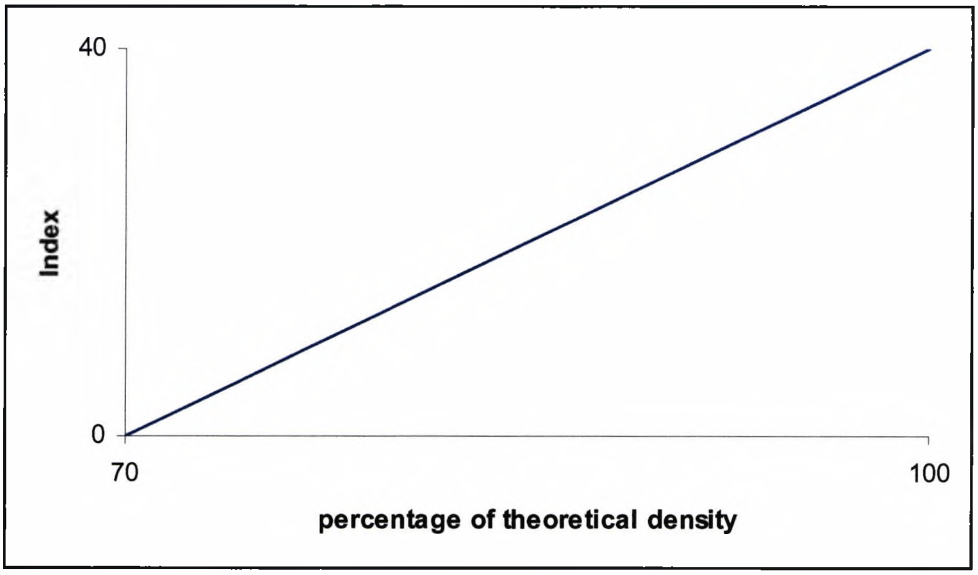


FIG. 8-5 Porosity Vs Index

(2) Thickness

The electrolyte is required to be as thin as possible to maximise ionic conductivity and minimise ohmic losses. The lower thickness limit is only dictated by mechanical requirements. For some of the solid oxide fuel cell configurations, Electro-vapour deposition and/or chemical vapour deposition are the techniques employed for fabrication. These techniques have enabled to make electrolyte layers thinner than 10μm.

In the particulate method, however, cell components must be made a lot thicker as they are supposed to be self-supporting. In the segmented-cell-in series design configuration, electrolyte thickness in the range of 110 – 150μm have been fabricated. This value allows for adequate strength and acceptable ohmic loss in the self-supporting configuration. Hence a thickness target of 110μm is given the maximum point (30 points) with the bottom extreme (0 points) being a thickness of 400μm in the index (Fig.8-6).

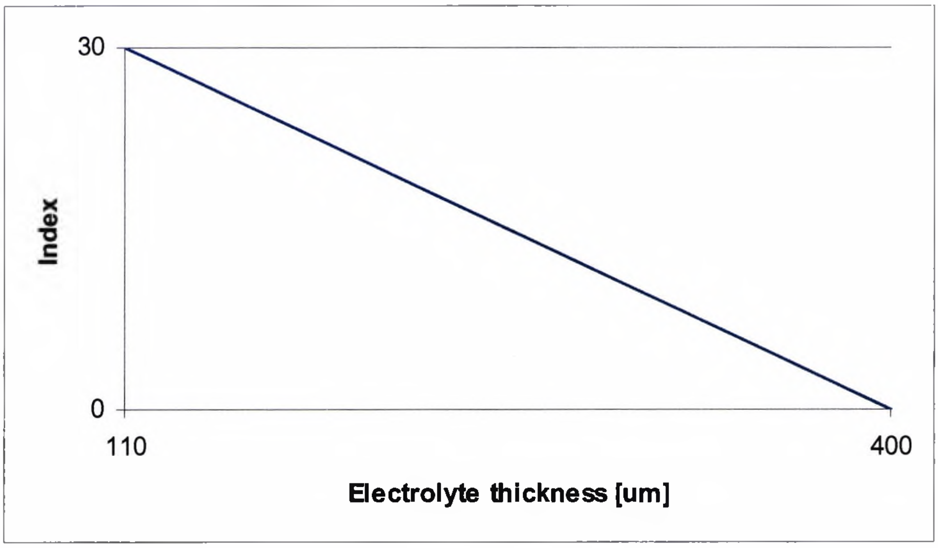


FIG. 8-6 Electrolyte Vs Index

(3)- Mechanical strength

Any cell component must be designed to an adequate mechanical strength for assembly and handling. The design must also satisfy other structural requirements created by the need to maintain good electrical contact between individual cell components in a leak-free manner. Thus, mechanical and thermal stresses must be kept to minimum to prevent cracking, delamination, or detachment of components under the variety of operating conditions.

The mechanical properties of YSZ electrolyte layer vary, depending on the characteristics of starting powders used in the fabrication (such as particle size, particle size distribution, and agglomerate strength) and fabrication route and fabrication conditions.

The bending strength and toughness are particularly important aspect of the required mechanical strength. Toughness as in fracture resistance greatly depends on the additives to the YSZ powder. The bending strength on the other hand, depends on the combination of material density and thickness.
The rupture stress is taken as a strength measurement, in this case. A value of 20 MPa, which is too low to stand the residual stress is assigned a score of zero points and 100 MPa the maximum score of 20 points. (Fig.8-7).

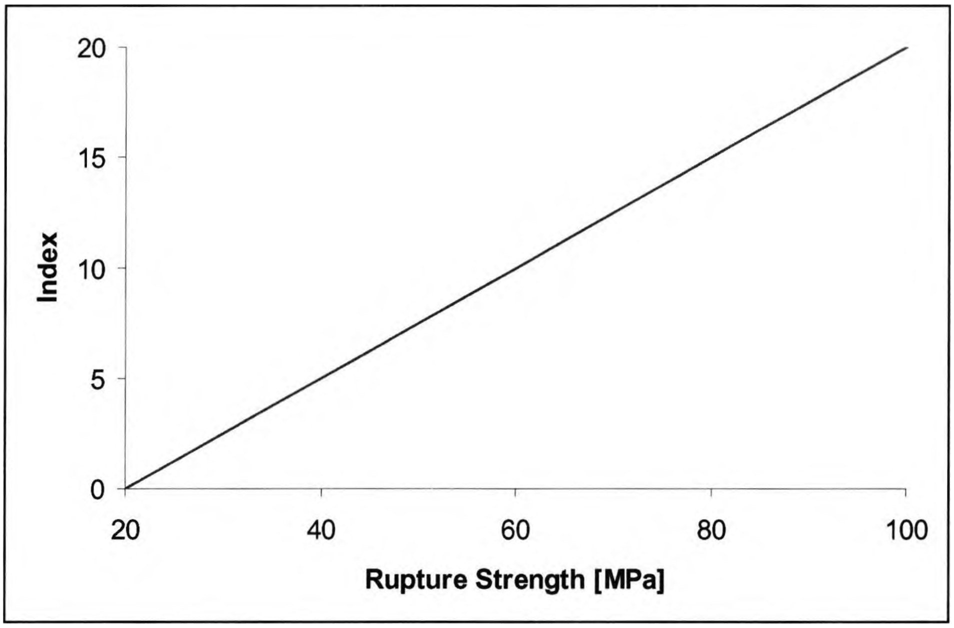


FIG. 8-7 Rupture strength Vs Index

(4) Cost

The variables in the fabrication process here do not cause much difference in regards to cost. The cost of materials used, however, does. In this experiment, two powder grades of yittra-stabilised zirconia are used. In this case, the index has only one value for each of the powder grades depending on their purchase price, with the coarse grade at a value of 7 and the fine powder at 5 out of a maximum 10 points in the index (Fig.8-8). These figures are nothing but relative values assigned by the designer.

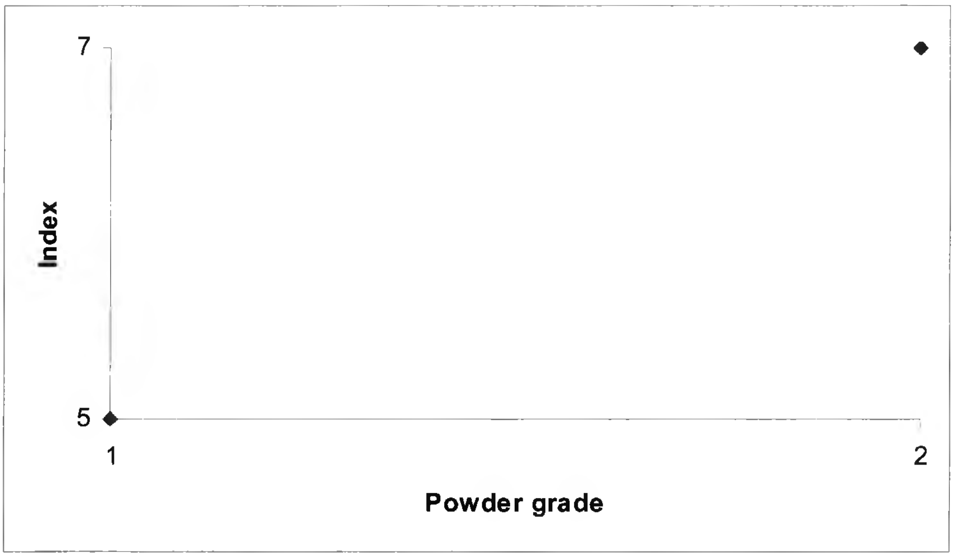


FIG. 8-8 Powder grade Vs Index

7.5- EXPERIMENTAL LAYOUT

The L_8 orthogonal array in Fig.8-9 was selected for the factors since it is the most efficient reduced orthogonal design to accommodate five factors at two levels. The L_8 array specifies eight experimental runs to be conducted, but the intention is to find the $2^5 = 32$ combinations that exist. This can be done since the design is orthogonal, a property that permits the effect of each factor to be separated out. The – and + signs in the array denote the first and second levels of a factor respectively. The first test condition in the L_8 array, for example, has all – signs across the row, dictating that all the factors should be set at their first level for that particular experiment. Three design changes at a time were made to form the complete parameter-design layout as shown in Fig.8-9. A two and four design changes at a time would result in 16 and 4 test runs respectively. The more test runs there are, the more accurate the prediction would be, and more expensive to conduct. The choice of three design changes is then a compromise between accuracy and cost.

	FACTORS				
RUNS	A	B	C	D	E
1	-	-	-	-	-
2	-	-	+	+	+
3	-	+	-	-	+
4	-	+	+	+	-
5	+	+	-	+	+
6	+	-	+	+	-
7	+	+	-	-	-
8	+	-	+	-	+

FIG.8-9 The $L_8(2^5)$ *orthogonal array*

8-6 RESULTS AND INTERPRETATION

In this experiment, the data is interpreted on the assumption that the effect of any one factor on the response is independent of the other factors. In other words, there are no interactions between the factors. The assumption can easily be verified by considering only two factors at a time and checking for possible interactions between them. That, however, falls above the allocated budget for the project.

Each process configuration is referred to as a *run*, so that in the first configuration (run 1 in Fig.8-9) all the factors are set at level-1. Three design changes are made at once rather than just one as in the one-factor-at-a-time approach. The experiment proceeds through to run 8, with levels of three factors being changed between each pair of runs. All the eight runs together make the experiment.

The parameters that determine the quality function of the washer shaped electrolyte fabricated at different conditions are measured and index values derived from the results.

The porosity of the electrolyte was measured from the difference of the weights of the specimen measured in dry condition and measured after being immersed in water. The level of moisture absorption is an indicator of the porosity percentage. This was compared with the porosity estimate from scan electron microscope (SEM) image analysis. Twelve specimens were obtained for every test run condition in the orthogonal array. An average porosity percentage for every test run comparing the two measurement techniques is presented in Fig.8-10.

Test run	Average Porosity (%) (using weight difference)	Average Porosity (%) (using image analysis)
1	79%	83%
2	80%	86%
3	85%	87%
4	92.5%	91%
5	93.25%	94%
6	94%	93%
7	92.5%	93%
8	88%	89%

Fig.8-10 Porosity data for the electrolyte at different sintering conditions.

The SEM image analysis showed a variation of 10% in the porosity measurement taken at different positions of a single specimen and 15% variation between specimens produced from the same sintering conditions. Whether this is due to non-uniformity of the density across the specimen or error in the analysis is unclear. A typical SEM micrograph image is shown in Fig.8-15. The weight comparison technique, however, gave a more consistent results of 4% variation in porosity between specimens of the same batch. The weight comparison technique is used for the analysis. The thickness of the electrolyte components were characterised using the SEM, and measurements of which are given in Fig.8-11.

Test run	Average thickness [μm]
1	293
2	282
3	226
4	168
5	177
6	158
7	168
8	235

Fig.8-11 Thickness data for the electrolyte at different sintering conditions.

Strength was considered as the rapture stress since the fracture stress is hard to detect. Fig.8-9 shows the average recorded stresses at failure.

Test run	Stress at rupture [MPa]
1	76
2	80
3	68
4	64
5	67
6	61
7	63
8	73

Fig.8-9 Average stresses at failure.

All the measurements for the porosity, thickness, and strength are then used to assign score values in relation to the index scaling (Fig.8-5 – Fig.8-8). This allows the quality defining parameters to be taken into consideration, depending on their corresponding importance rating, to derive the quality rating of the product. In this case, electrolyte performance.

	FACTORS					QUALITY FUNCTIONS				
RUNS	A	B	C	D	E	Pi	Ti	Si	Ci	ΣQF
1	-	-	-	-	-	12	11	14	7	44
2	-	-	+	+	+	13	12	15	7	47
3	-	+	-	-	+	20	18	12	7	57
4	-	+	+	+	-	30	24	11	7	72
5	+	+	-	+	+	31	23	12	5	71
6	+	-	+	+	-	32	25	10	5	72
7	+	+	-	-	-	30	24	11	5	70
8	+	-	+	-	+	24	17	13	5	59

FIG.8-13 Experimental plan and test results

The purpose of statistical analysis in the experimental context is to try to relate the variation in the response directly to the changes in the factor levels. The results have been arrived by evaluating the quality functions individually and assigning values to them. Porosity, for example, was measured by weighing the component both in water and air to establish the water absorption, which in turn indicates the level of porosity. The fact that run-6 resulted in a higher value of the quality function compared to the other test runs in the L_8 experimental layout does not mean that it is the best combination. Each factor has to be evaluated. The best combination might well be outside the eight test-run combinations conducted from possible 32 combinations. The idea behind statistical experimentation is to obtain knowledge on the effect of the factors at lesser experimental runs. In other words achieving quality at a lower cost.

The impact of each of the factors is evaluated by first calculating the average value of the quality function when that factor was at level-1 and compare it to when the factor is at level-2. The difference of the two values measures the effect of the factor on the product's quality.

It might be true that run 6, with the highest quality function value, produced the best result of all the eight test runs. But it is not necessarily the best combination possible as only eight combinations out of possible 32 are being analysed. The idea, therefore, is to analyse each of the factors' influence on the overall quality function.

The quality function is rated out of hundred, the higher the better. Fig.8-14 compares the average value of the quality function when the factors are at level 1 and level 2. Many conclusions can be deducted from the results. One important point is the choice of factor levels to achieve a better quality function. Take factor A, for example, the average value of the function at level-1 (using coarse powder) is 55% and is 68% when A is at level-2 (fine powder). This is an indication of the fact that using finer powder yields a superior quality compared to the coarse one. If the same analysis is extended to the other factors, one can see that a choice of fine powder, with a compaction force of 6 kN, sintering temperature of 1600^{o}c, and sintering time of 16 hrs, cooled in the furnace (A+,B+,C+,D+,E-) is the best combination. This combination is not among the eight test runs but was made possible to be picked as an optimum one thanks to Taguchi's statistical experimentation. One can then claim that quality has been improved at reduced cost. The other conclusion that can be made from Fig. 8-14 is which factors play a dominant role in the quality of the product. This is indicated by the difference between the averages of the values of the quality function at the two levels. With the highest difference in the values, between the two levels, the powder grade most influences the quality of the product.

It is, however, imperative that the conclusion one makes must be incorporated with engineering knowledge and experience. Experiments must also be run more than once to avoid human and other sources of possible error.

FACTORS	AVERAGE AT LEVEL-1	AVERAGE AT LEVEL-2
A	54.50	72.25
B	55.50	71.25
C	62.25	64.50
D	58.50	68.25
E	67.50	59.25

FIG.8-14 Test results of the factors

The experimentation process involved two stages: first, a test on manufacturability was conducted, and second, a statistical experimentation was conducted on the selected fabrication procedure to analyse the factors involved.

The first experimentation (on conical and flat plate YSZ electrolytes) did not only help achieve the best manufacturing process towards quality improvement but also the cost and manufacturability of the different configurations. As a clear demonstration of concurrent engineering, manufacturing was not delayed until the completion of the design process, which would result in a design change at a later stage. This would cause unnecessary delay and extra cost. As was demonstrated in chapter 4, ease of the components fabrication played a dominant role in selecting the better cell configuration. In other words, information gained at the manufacturing stage was given back to the design process.

The second stage of experimentation (the Taguchi type statistical experimentation) enabled to achieve knowledge on performance at a reduced cost. It also enabled quality control and inspection to take place during the process itself unlike in the traditional *after the product inspection* method, which is rather costly. The test demonstrates that the advantage and cost effectiveness of this procedure becomes apparent when many more factors, such as different materials and manufacturing techniques are involved. The cost reduction in such an experiment with more factors and levels is significant in the development of a product.

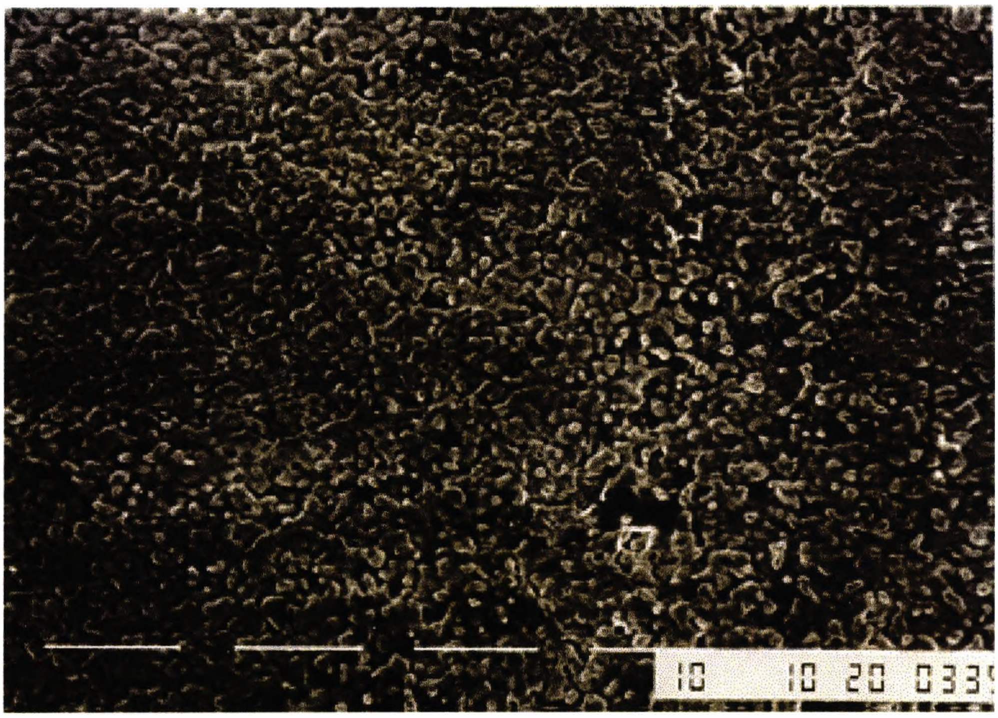


FIG.8-15 Microstructure of fine powder YSZ sintered at 1500^{o}c

CHAPTER-9
DESIGN OPTIMIZATION

9.1- INTRODUCTION

Design optimisation is a process where values are chosen to the design parameters in order to obtain the best design. At the optimisation stage in the design process, one has to reach a decision for the selection of discrete value dimensions and operating variables.

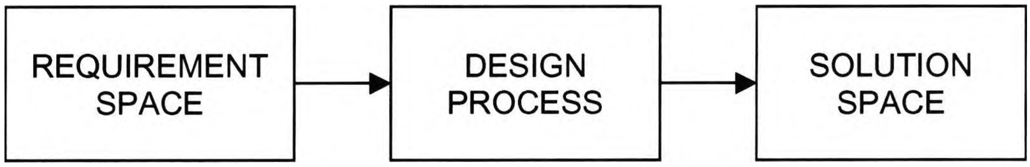
Practical problems of optimum design are not simple in nature. First, the engineer must recognise the critical areas of design where optimisation techniques are likely to pay off in the result achieved. Secondly, he must be able to formulate the optimisation problem, not only from the standpoint of the optimisation quantity itself but also from the standpoint of the subsidiary quantities, specifications, and various constraints. Finally, he must be able to handle the system of equations thus formulated, drawing design conclusions of value from the variation study mode, which can be applied to the problem at hand. Hence, we see that application of optimum design in a realistic decision-making process requires an understanding of optimisation theory integrated with engineering science, practical experience, design talent, and good engineering judgement.

The following aspects show the necessity of introducing optimisation procedures into the practical design phase:

1- Increasing the quality and quantity of products and plants and at the same time reducing costs and thereby being competitive.
2- Fulfilling the permanently increasing specification demands as well as considering reliability and safety, observing severe pollution regulations and saving energy and raw materials.
3- Introducing inevitable rationalisation measures in development and design offices (CAD, CAE) in order to save more time and get the design right the first time round.

9.2- DESIGN PROCESS

The act of designing is divided into two spaces, the requirement space and solution space mapped by the design process.



The solution space is the area where visualisation of the entire spectrum of viable solutions is made and an optimum one identified.

It has been explored in the previous chapters how a design function deployment can be useful in retrieving information on the design procedure. It was also demonstrated how DFD helped identify interactions between design functions. This methodology, however, has its limitations on the area of solution space. Having identified the interaction between parameters, it does not indicate the direction of influence. DFD has the difficulty integrating mathematical findings with the design procedure and interactions.

In this chapter the information stored on the DFD charts is taken a step further to integrate the mathematical results with the parameters. The direction of influence among the parameters will be established in order to work out which parameters are fixed and which are within an iterative loop to determine the optimum design parameters.

9.3- DESIGN PARAMETERS

Design parameters are all the variables that affect the overall performance of a product. A designer has to assign values to these variables at the solution space. This is an important stage of the design procedure as the values usually determine the quality of a product. The need for design optimisation becomes apparent where many interdependent parameters are involved. The following is a list of parameters in the design of solid oxide fuel cells.

A- *Active surface area*. The area the electrolyte and electrodes overlap where the current is generated.

B- *Interconnect length*. The smaller it is, the better to shorten the current path there by reduce ohmic losses.

C- *Electrolyte thickness*. An important parameter that strongly influences the electrochemical performance of the cell.

D- *Cell diameter*. Determines the active surface area.

E- *System efficiency*. The yardstick of cell performance, It is a parameter one hopes to maximise.

F1- *Cathode thickness*. The smaller the thickness, the less losses due to Ohmic polarisation.

F -*Anode thickness*. The maximum size is dictated by electrical requirements While its minimum limit is dictated by mechanical requirements.

G- *Fuel utilisation %*. The percentage of the fuel entered in a single cell that is Consumed. The practical maximum is 85%.

H- Length of air flow path. This depends on the number of cells in parallel (or the required power), manifold design and fluid flow considerations.

I- Current density. An important value that will determine the efficiency of the stack.

J- Rate of fuel flow. This parameter can be adjusted to determine the percentage consumption and in turn depends on the required power.

K- Rate of oxidant flow. The air flow has two purposes; to heat the entire system and supply oxygen to the cathode.

L- Number of cells in series (stack). Cells are added in series to build the voltage.

M- Manufacturing constraint. This parameter affects the cell geometry.

N- Number of stack in parallel. The number of stack grows to meet the required power.

O- Stress distribution. This is mainly due to differential expansion mismatch.

P- Required power output. This parameter is set initially as a requirement.

Q- Power per weight ratio (specific power). Sometimes referred as power density. The higher it is, the more compact the system is.

R- Internal cell resistance. The smaller the cell resistance the better the cell performance.

S- Sealing mechanism. A design mechanism that differs from one conceptual design to the other.

T- Cell working temperature. This value is set by the cell material properties (conductivity etc.)

U- Rate of reaction. This greatly depends on the operating temperature and the cell materials used.

V- Cell operating voltage. An important value coupled with the current will determine the efficiency of the stack.

W- Inlet pressure. The pressure required to pump the working fluids through *The system.*

X- Start up time. The time needed for reaction to begin at the operating temperature.

Y- Carbon deposition. This degrades cell performance by reducing the Diffusion rate.

Z- Working life of cell components. It is the reliability of individual cell Components under the working conditions.

α- *Cost of fabrication*. This includes the cost of material and its manufacturing technique.

θ- *Material for cell components*. The choice of materials greatly depends on the required properties and working temperature.

β- *Cross sectional area of fuel flow*. Depends on the cell geometry.

Δ- *Cross sectional area of air flow.* Depends on the stack length and their numbers in parallel.

9.4- PARAMETER CORRELATIONS

A square correlation matrix proposed by Atherton [11] as a replacement to the triangular roof of the QFD matrix is used. This is because; the triangular matrix does not indicate the direction of influence between parameters. For example, information like degree of interaction between two design functions 'A' and 'B' can be stored. Negative interaction would imply the need for trade-offs. It is however, important to avoid trade-offs where possible as they are performed at the expense of one design function or another. A square correlation matrix makes this possible by identifying whether parameter 'A' determines 'B' or viseversa. It gives way to the optimization process by integrating a mathematical solution to the design process.

The parameter correlation network in Fig(9-1) shows the direction of influence among the variables. Here all the design parameters are considered one by one. The initial network of correlation chains is simplified as given in Fig(9-2). Some of the links at the initial stage are redundant. For example, electrode thickness (F) determines the rate of reaction (U), which in turn determines the system efficiency (E). The link between (F) and (E) can then be eliminated as redundant. Some links are stronger and more direct than others. Hence care must be exercised in selecting the redundancies in the simplification process.

The next stage in the optimisation process is to determine the hierarchy of the correlation chains. At this stage, the choice of values to parameters is made. Fixed or independent parameters are set at the initial stage to be followed by the variables directly determined from the fixed parameters. It goes on stage by stage in the hierarchy depending on the variables dependence on others. Parameter P, T and M appear to be independent of other parameters and are set at the first stage in the ten-stage hierarchy. This does not mean, however, that the parameters are totally independent of others. Power output (P), for example, depends on many design variables, but is fixed at the initial stage as a requirement.

Parameters like inlet pressure (W) and efficiency (E) are determined at the final stage in the hierarchy. This indicates their dependence on many other parameters. Inlet pressure depends on rate of oxidant flow and the geometry, which are also determined at the later stages. The efficiency, on the other hand, is influenced by many variables thus placed at the final stage. It in turn influences other parameters such as the number of cells in a stack (L) up in the hierarchy to create iterative loops. The choice and/or calculation of variables continue in an iterative manner until an optimum design is achieved.

The network is rewritten in a matrix format in Fig(9-5). Unlike the triangular matrix, the relationships in the square matrix can be classified into rows and columns depending on the direction of influence. Parameter A for example, is influenced by parameters D, L and G indicated across the A-column and influences parameters I and Q indicated across the A-row. The symmetrical nature of the square matrix gives it an extra dimension to store that more information.

9.5- PARAMETER HIERARCHY

All the design parameters are divided into four groups containing: the fixed parameters, free design variables, calculated design variables, and design targets. Each of the parameters in the groups is determined in a descending order in the hierarchy.

A- **Fixed parameters** are those the designer needs to fix at the start of the process as design specifications. In this case, the required output, working temperature and manufacturing constraints are determined at the start of the design and optimization process.

B- **Free design variables** The name might be misleading as these variables are not entirely free, but depend on the already determined design specifications. Here, the variables are more or less the geometry of the product. The designer can alter the values of these parameters to bring about change in the subsequent variables in the hierarchy. For example, electrolyte or electrode thickness can be altered to optimize for mechanical and/or electrochemical performances such as internal cell resistance and rate of reaction.

C- **Calculated design variables** There isn't always a clear-cut landmark to divide the *free* from the *calculated* design variables. These variables are determined mathematically from the choices made to the parameter values at the previous stage. Such variables, in this case, are the fuel consumption and current density which are calculated from the number of cells and active surface area which, in turn, were set values at the previous stage as a free design variables.

D- **Design targets** These are the target values the designer sets as quality assurance exercise. They are the values that are determined qualitatively, i.e., maximizing or minimizing the values as much as possible. One doesn't necessarily assign values to these parameters. In this case study, maximum power per weight ratio, maximum efficiency, minimum carbon deposition, minimum start up time, longer working life of components, and more importantly minimum cost of fabrication constitute the target design parameters.

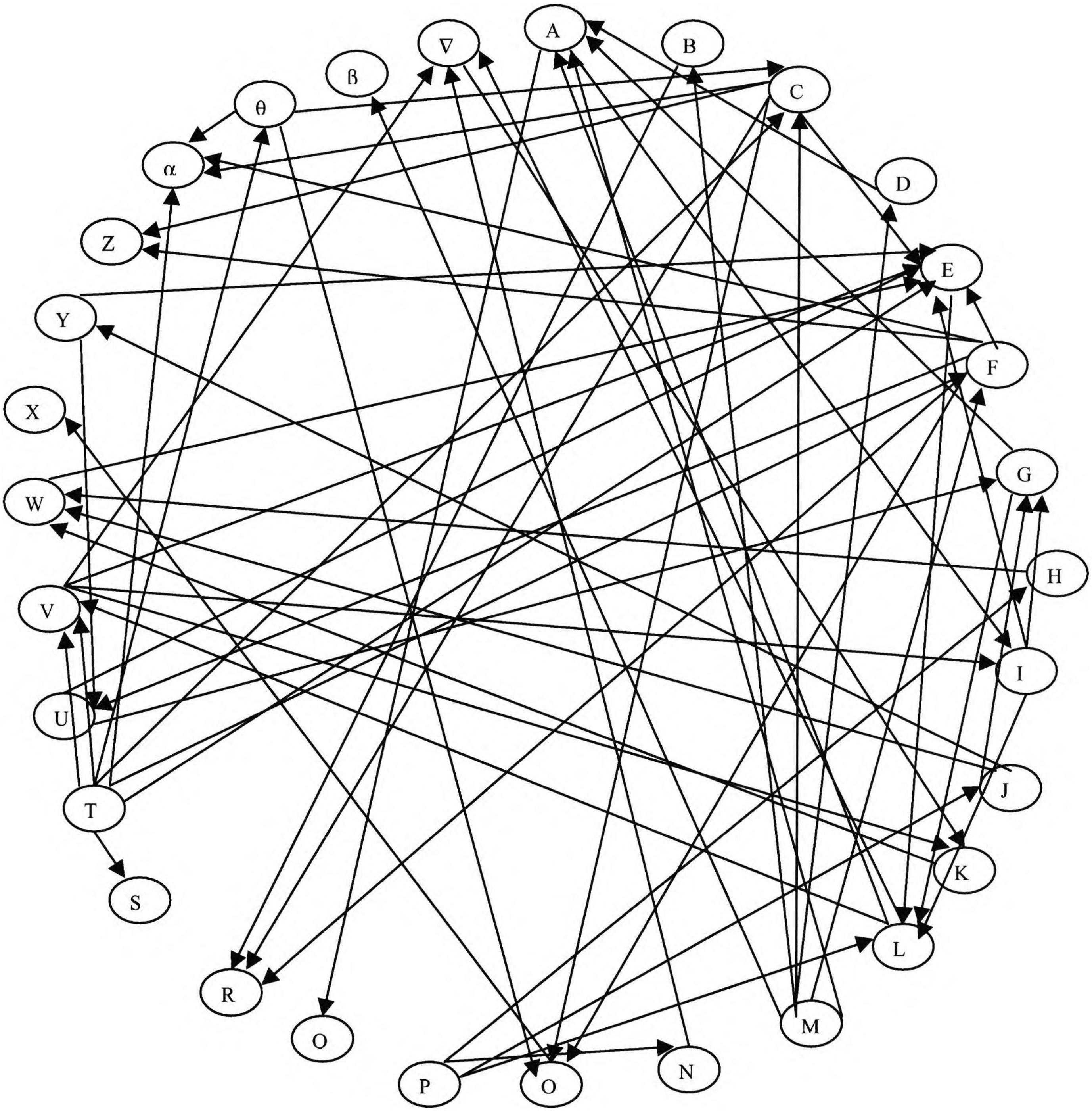


FIG. 9-1 Network of correlation chains

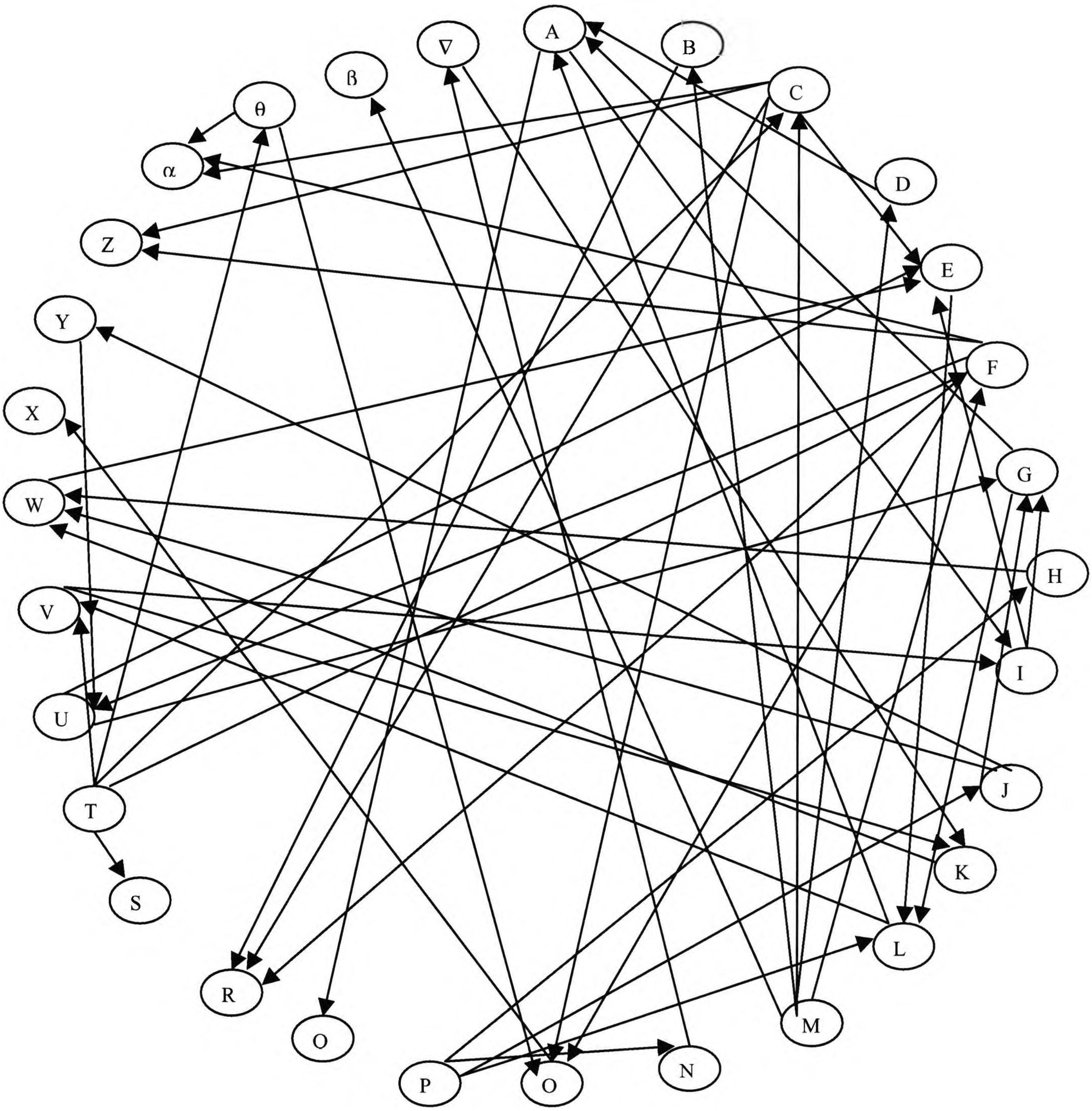


FIG. 9-2 Reduced Network of correlation chains.

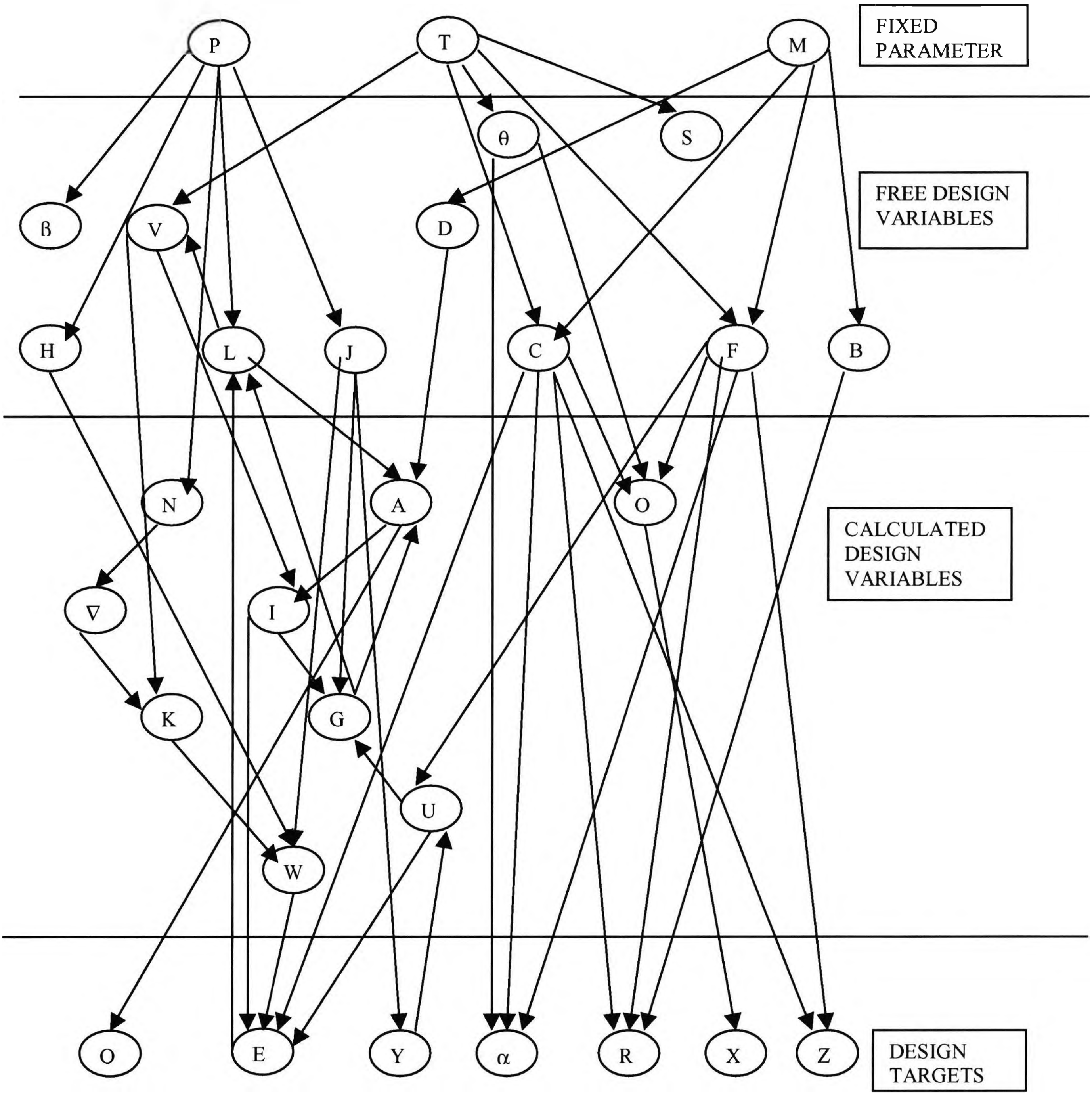


FIG.9-3 Correlation chain network hierarchy

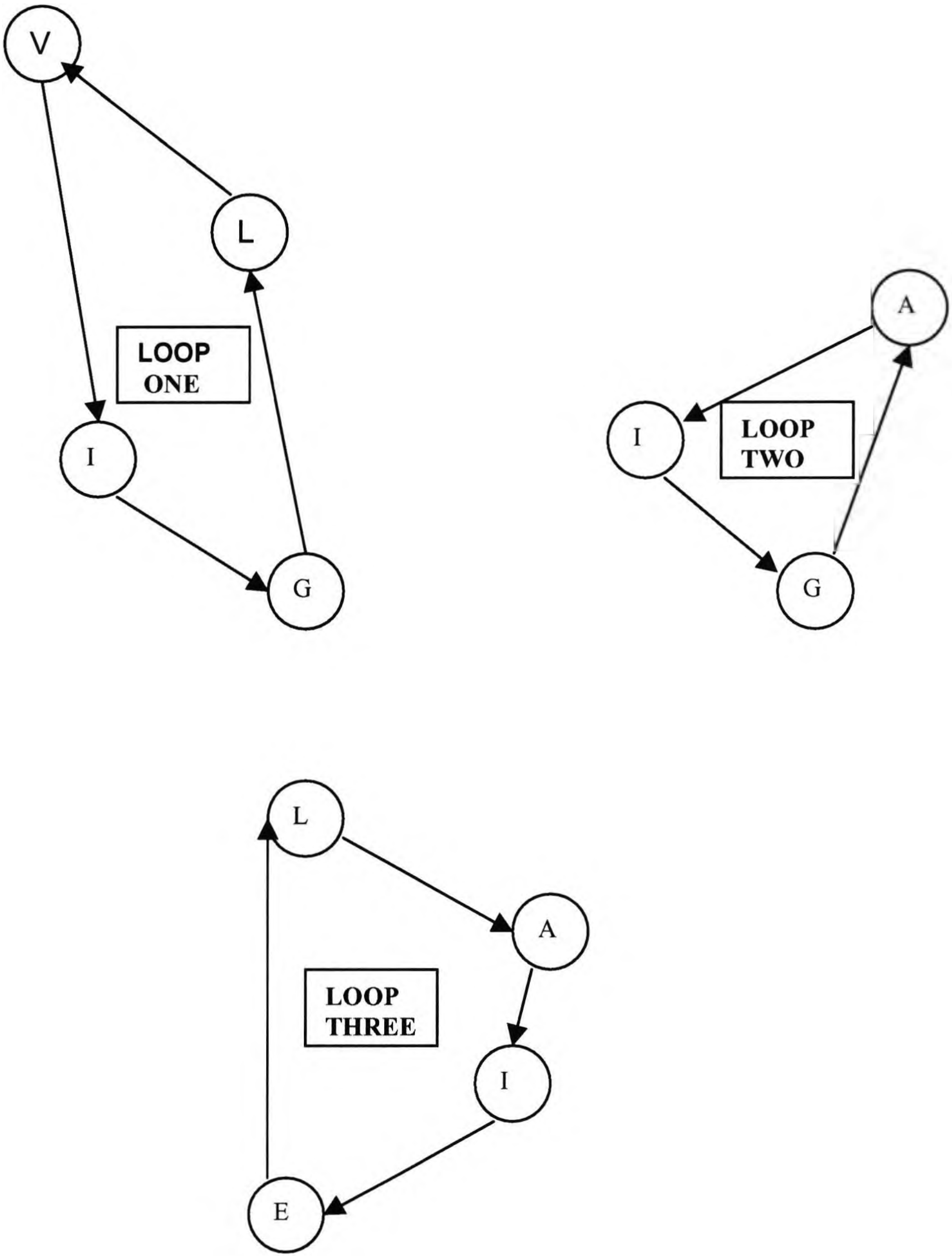


Fig. 9-4 Iteration loops.

	P	T	M	θ	S	β	V	D	H	L	J	C	F	B	N	A	O	∇	I	K	G	U	w	Q	E	Y	α	R	X	Z	
P	▨					*			*	*	*				*																FIXED PARAMETERS
T		▨		*	*		*					*	*																		
M			▨					*				*		*																	
θ				▨													*										*				FREE DESIGN PARAMETERS
S					▨																										
β						▨																									
V							▨												*	*											
D								▨								*															
H									▨														*								
L										▨						*															
J											▨												*			*					
C												▨					*								*		*	*		*	
F													▨				*					*					*	*		*	
B														▨														*			
N															▨			*													CALCULATED DESIGN PARAMETERS
A																▨			*					*							
O																	▨												*		
∇																		▨		*											
I																			▨		*				*						
K																				▨			*								
G										*						*					▨										
U																					*	▨			*						
W																							▨		*						
Q																								▨							DESIGN TARGETS
E										*															▨						
Y																						*				▨					
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VERTICAL = STARTING POINT VARIABLES
HORIZONTAL = DERIVED VARIABLES

FIG.9-5 Square matrix of the correlation chain proposed for the roof of the house of quality.

9.6- SOLUTION SPACE

Unlike the traditional QFD or DFD charts, the square correlation matrix records the essential information of the direction of influence between the parameters. For it to incorporate the laws of physics or engineering science and reduce the solution space, however, it needs to be modified in such a way that the parameters are categorized into fixed parameters, free variables, derived variables and target values. Parameters are recorded in a form of hierarchy starting with the specification (fixed parameters) down to the design target values in the square replacement for the roof of the house of quality. Here, not only are the interactions between parameters established but also the direction of influence between parameters to dictate which parameters need to be determined first. Moreover, the stages where mathematical models and experimental results are used can easily be identified.

The experience gained from the Taguchi type experimentation, together with common engineering knowledge are used at the free variables stage of the hierarchy. At this stage, materials used are chosen and values are given to electrodes and electrolyte thickness, cell diameter, interconnect length, etc. The values given to these parameters are fed to the mathematical models (electrochemical, fluid flow and thermal stress models in this case) to calculate the next set of parameters in the hierarchy. Some of the interactions in the square matrix (Fig.9-5) fall below the diagonal. This indicates some of the down stream parameters influence those at the upstream, which usually forms iterative loops as in Fig.(9-4).

The electrochemical model have produced that a 3 cm diameter cell with 7 cells in series to form the stack was the most efficient combination for a given fuel utilization percentage (85%). This conclusion was derived from loop number three, where different practical values for the cell diameter were assigned and an optimum one identified. The current generated increases as the cell diameter increases, but for fixed fuel flow and utilization percentage, the increase in surface area limits the number of cells in series which means limiting the stack voltage which is the sum of individual cell voltages in series.

Since power is directly proportional to current and voltage (Fig.6-5 & 6-6), the increase in current increases the power up to cell diameter of 3 cm, beyond which power starts to drop as the increase in current does not make up for the loss in stack voltage. Fig.9-6 compares the results for all the assigned values at a fuel flow rate of 11 L/hr, and typical fuel utilization percentage of 85%.

Cell Diameter[cm]	Number of cells in a stack	Current generated[A]	Voltage in a stack [v]	Power[w]
2	17	1.03	12.75	13.13
3	7	3.04	5.25	15.96
4	4	4.51	3.00	13.53
5	3	5.95	2.25	13.39

Fig.9-6 Results of Current, Voltage and Power under different conditions.

Similarly, the same iteration is performed in the other loops and all other direct calculations to determine the optimum parameters for an optimum cell performance. The last stage of optimization procedure consists of the design targets. Here, any optimization criteria can be chosen. Whether it is just maximizing the efficiency as in the case above or reducing carbon deposition, maximizing reliability or even a combination of all the design targets depending on the designer in order to satisfy customer and design requirements. A combination of all the design targets depending on their importance rate is the ideal optimization criteria (Appendix-C). The above loop, however, was independent of the other design targets, and iteration was only aimed at maximizing efficiency or the power at a given fuel flow rate.

The correlation network suggested a design optimization strategy, but was considered most useful in identifying dependent and independent variables. Construction of the hierarchical correlation chains gives a much better insight into the problem. It has been seen that the approach is, modeling a combination of the design team's working knowledge and experience of the underlying engineering science.

The correlation chain network hierarchy in Fig.9-3 is not unique. The direction of influence can be arguably different in some cases. For example, the interaction between the current and voltage can be in either direction. As shown in Fig.6-6 and Fig.6-8, the values of these two variables affects the efficiency. Which ever way the calculation is done, i.e., either starting from the value of the voltage to determine the current (as in the electrochemical model), or starting from the value of current to determine the voltage would make no difference to the target values. If, on the other hand, efficiency was not considered a target value, but a fixed parameter, we would end up with different set of parameter values. So care should be exercised particularly in determining the target parameters as they dictate most of the other free and derived variables.

10- CONCLUSION

The milestones in this project can be categorised in to two: 1- its contribution to the design methodology, and 2- its contribution to the solid oxide fuel cell technology. The DFD methodology has been taken a step further to accommodate complex design problems involving complex mathematical equations. The study has also produced a design rule for solid oxide fuel cells by combining mathematical models, manufacturing analysis in a concurrent engineering approach.

Atherton's proposed square replacement for the roof of the DFD matrix, in order to link the voice of customer with engineering science, only works to a point. It helps record the direction of influence between parameters, but the parameters need to be categorised into four groups of design requirements, free design variables, derived variables, and target parameters as in Fig.10-1, in order to simplify the optimisation process and achieve a mathematically optimised solutions. This is done by identifying an optimisation criteria from the target parameters. The optimisation criteria depends on whether one is designing for cost, efficiency, reliability, manufacturability, etc. Ideally, one would like to design for all the above parameters, but in real world, these parameters are often compromised with each other and prioritisation becomes essential. The methodology enables the designers to derive an optimisation criteria from the combination of the target parameters to build a complete design methodology.

Making use of correlation chains, which can be recorded, in the modified square correlation matrix (chapter -9), it was possible to identify the solution space for the mathematical models and calculate optimum dimensions and working parameters for the fuel cell. The square matrix (Fig.10-1) can be decomposed into a set of design rules and contains a design procedure or methodology for a particular design problem.

Classification of the parameters into the four groups is subjective and by no means unique. Different designers faced with the same parameters might select different classifications. Nevertheless, it is proposed that all problems should have some design requirements, free variables, derived variables and target parameters. This should be universal to any design problem and should form an essential component of any generic design methodology. The existence of a universal methodology and mathematically derived optimum for any engineering design, however, remains unproven.

The design exercise produced a design rule and a new cell configuration for solid oxide fuel cells, named by the author, a combined cell configuration. The name suggests that the design was a combination of the already proposed cell configurations. All the conceptual designs were analysed on the same matrix using DFD charts and Taguchi experimentation. These were compared for qualities like, efficiency, ease of fabrication and lower cost of manufacturing. The combined design uses planar cells, which are relatively cheaper to make and avoids the sealing problem associated with the planar cell configuration by introducing a tubular interconnect. The advantages, however, do not come with out a cost. The combined cell configuration is potentially less efficient than the planar cell design due to high ohmic losses induced by longer current path which in turn is caused by the tubular interconnect. Whether or not, the lower cost of fabrication achieved in this design makes up for the loss in efficiency, depends on the intended application of the product. For a micro CHP (combined heat and power) where the plant is to be used in supplying heating and electricity for apartments, the combined cell can be the choice of the cell design, where as the product is used for high efficiency space applications, cost becomes a distant second and more efficient cells might be applied. Detailed design of the combined cell configuration is given in Appendix-A.

A new cheaper fabrication route for the electrolyte based on constrained sintering on a cement rigidized alumina paper is achieved. This brings down the cost of fabricating planar electrolyte, which was a dominant factor in determining the geometry of the proposed conceptual design. Reducing the cost of fabrication will certainly play an important role in bringing the solid oxide fuel cell state of the art to commercial reality.

The experimental results did not only help achieve the best manufacturing process towards quality improvement but also the cost and manufacturability of the different configurations. As a clear demonstration of concurrent engineering, manufacturing was not delayed until the completion of the design process; it was rather a parallel activity with 'to' and 'from' flow of information. In this case, cost and ease of the components fabrication played a dominant role in selecting the better cell configuration. In other words, information gained at the manufacturing stage was used to make decisions at the design stage.

The Taguchi type statistical experimentation enabled to achieve knowledge on performance at a reduced cost. It also enabled quality control and inspection to take place during the process itself unlike in the traditional after the product inspection method, which is rather costly.

From this study, it is not possible to estimate to what extent the DFD methodology contributed towards the design process. To check whether or not the achievements in the design process are attributed to the methodology itself, requires an extensive study. It requires testing with different groups of designers some of whom using the methodology, and the others with out it. Even then a conclusion might not be easily made, as there are other factors involved such as the individual skills, creativity and engineering knowledge of the designers etc. The DFD methodology is, however, invaluable in that the entire design experience is recorded for future reference. With the research and development on possible ceramic fuel cell components, many down stream design changes are inevitable. Some of the experience gained here can readily be recorded and retrieved through the existing DFD charts. It can clearly show how the design process was conducted and can identify where the subjective elements are, as any design problem involves subjective elements. For example, the weighting factors assigned to cost, manufacturability, efficiency etc. are subjective. They can be altered depending on the application of the product and the state of the art at a future date. The DFD methodology also serves as a focusing aid, but certainly not as a replacement for creativity and designers skills.

Electrochemical model (Appendix-C) gives us the basic scientific equations, which govern the fuel cell operation. Appendix-A shows the conceptual design of cell and stack configuration. The use of the modified square correlation matrix (Fig.10-1) linked the voice of customer with engineering science. The design parameters for appendix -A can now be related to the electrochemical model. It gives a clear optimisation strategy for searching the solution space. This can not be done with the conventional QFD triangular roof of house of quality.

The model predictions are used to determine the cell geometry, air and fuel flow rates and to evaluate the effect of varying design and operating parameters on the overall cell performance. The model results are by no means a replacement for experimental data. They, however, reduce the need for extensive experimentation before knowledge on performance is obtained. In other words, this is in line with the philosophy of achieving a quality product at a lower cost by reducing down stream design changes.

The electrochemical model has demonstrated the need for and usefulness of stack performance curves to accurately predict solid oxide fuel cell characteristics in a realistic power system. With out these curves and data, accurate assessments of the power per cell or stack and other important parameters could not be determined. The degree of accuracy of these predictions can not be determined until after a rig is built and tested. The model, nevertheless, is aimed at improving knowledge of cell performance at the design stage and to determine the design and input parameters.

The stage by stage hierarchy techniques has also made it possible to identify which mathematical model or design tool is used where. Information gained from the Taguchi experimentation, for example, was used to determine the free design variables in the hierarchy as indicated in Fig(10-1). These are mainly the geometric parameters that are influenced, predominantly, by the manufacturing criteria.

The mathematical models (electrochemical, fluid flow model and reliability) and manufacturing study (using taguchi type experimentation) were used as design tools in improving knowledge of performance of the cell hence dictating the design solutions. The methodology provides the platform where all these tools can be used to get an optimum solution to the design problem.

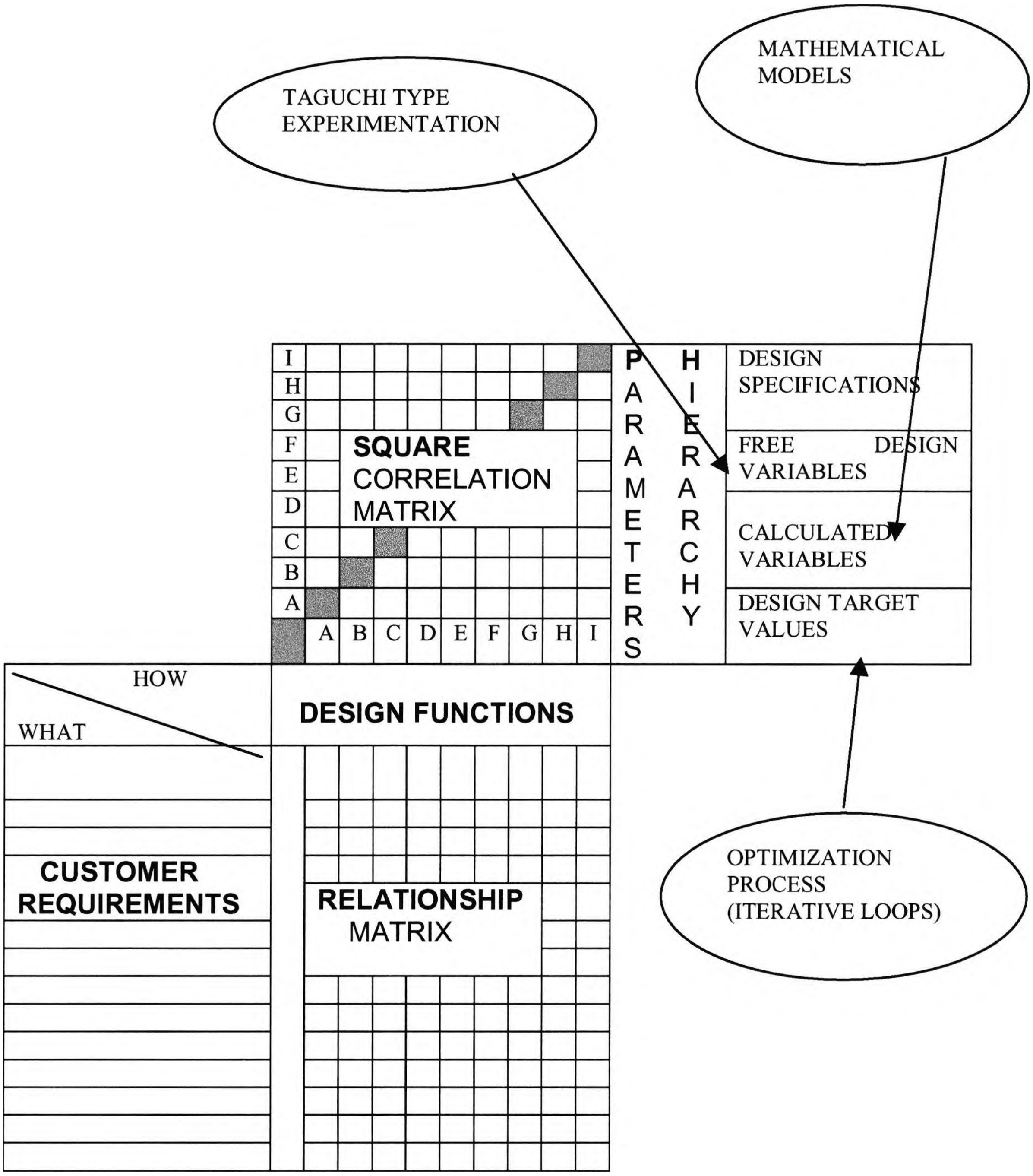

Fig.10-1 Proposed design chart for optimisation strategy.

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APPENDIX – A CELL AND STACK ASSEMBLY

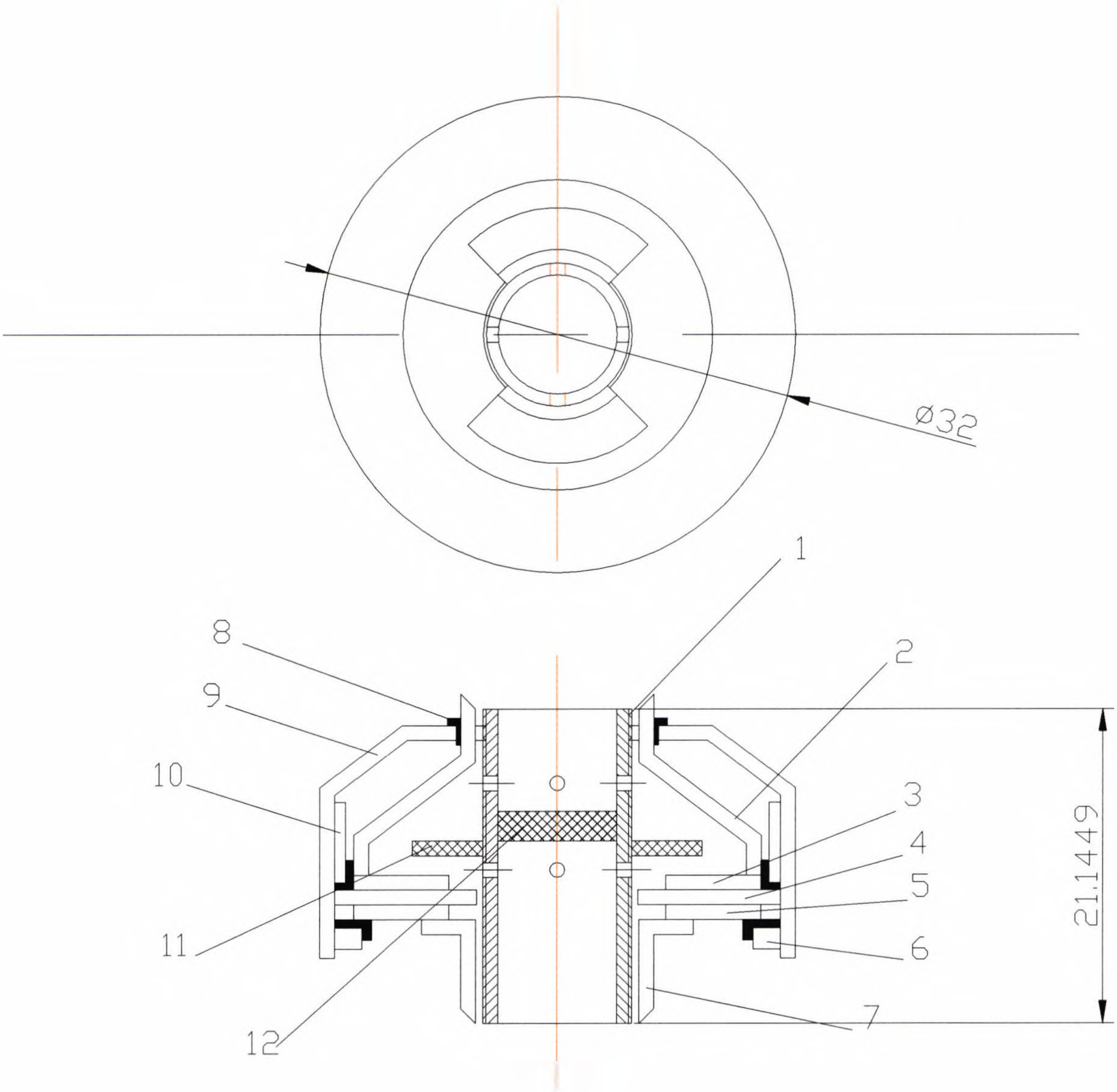

Fig.A-1 A unit cell of the combined SOFC configuration

Number	Function	**Material**
1	Fuel manifold and mechanical support	Fire bar ceramic
2	Interconnect	Inconel 600
3	Anode	Nickel cermet
4	Electrolyte	Yittra stabilised Zirconia
5	Cathode	Lanthanum manganate
6	Support ring	Inconel 600
7	Interconnect	Inconel 600
8	Insulating material	Alumina paper
9	Mechanical support	Inconel 600
10	Support ring	Inconel 600
11	Buffer plate	Fire bar ceramic
12	Buffer plate	Fire bar ceramic

Fig.A-2 Materials list of cell components

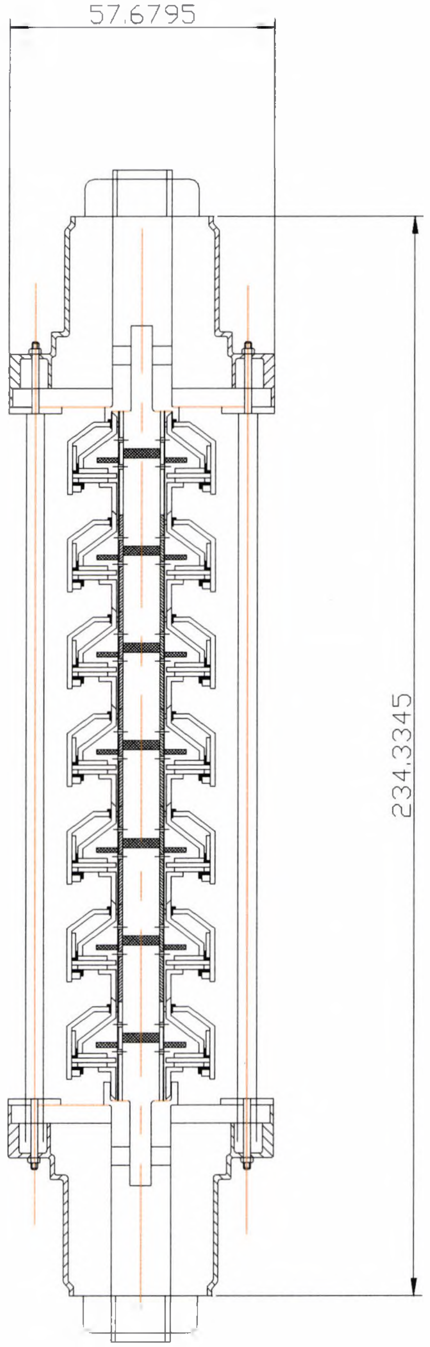

Fig.A-3 A combined SOFC stack

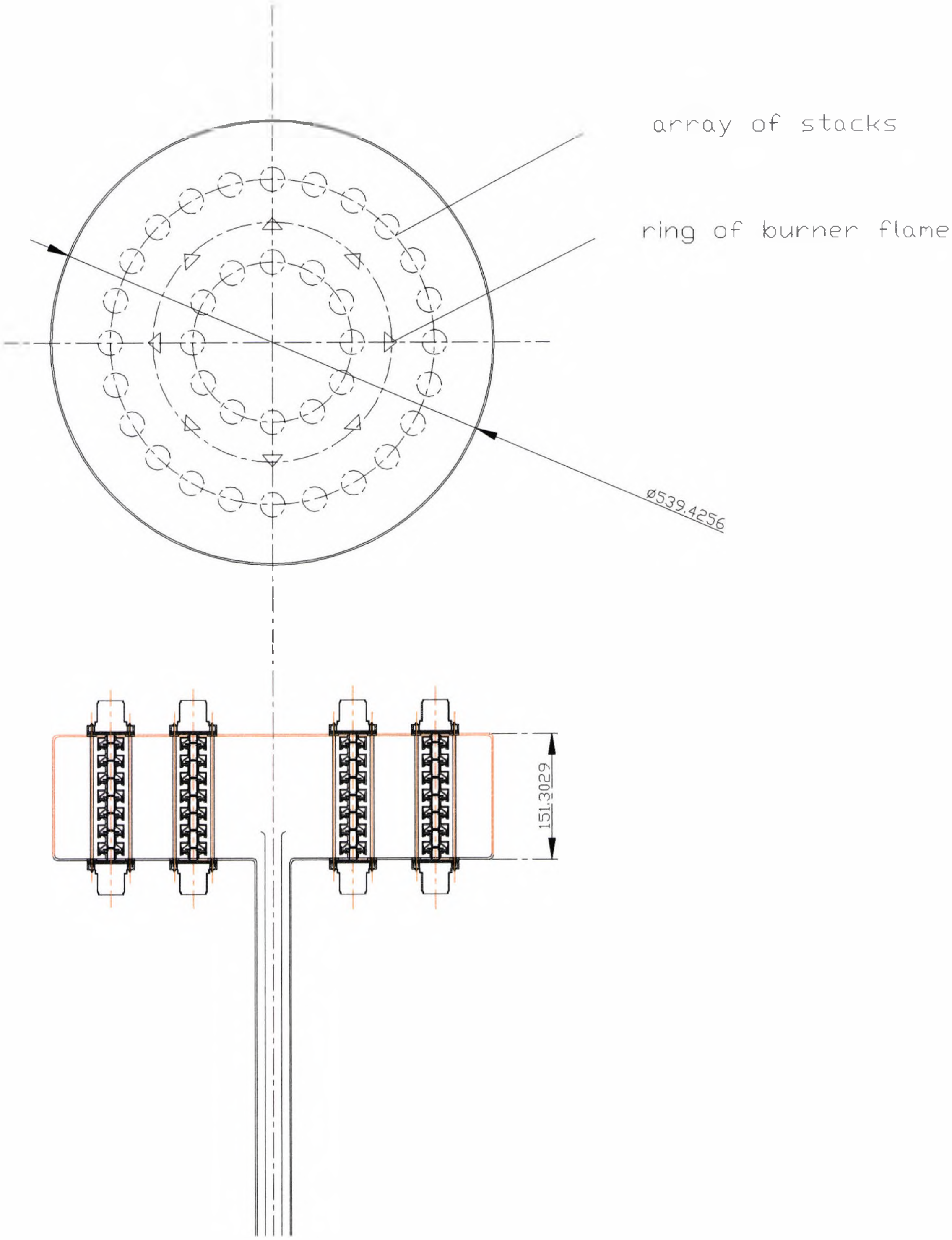

Fig.A-4 Manifold design of a 50 watt SOFC device based on the combined cell design

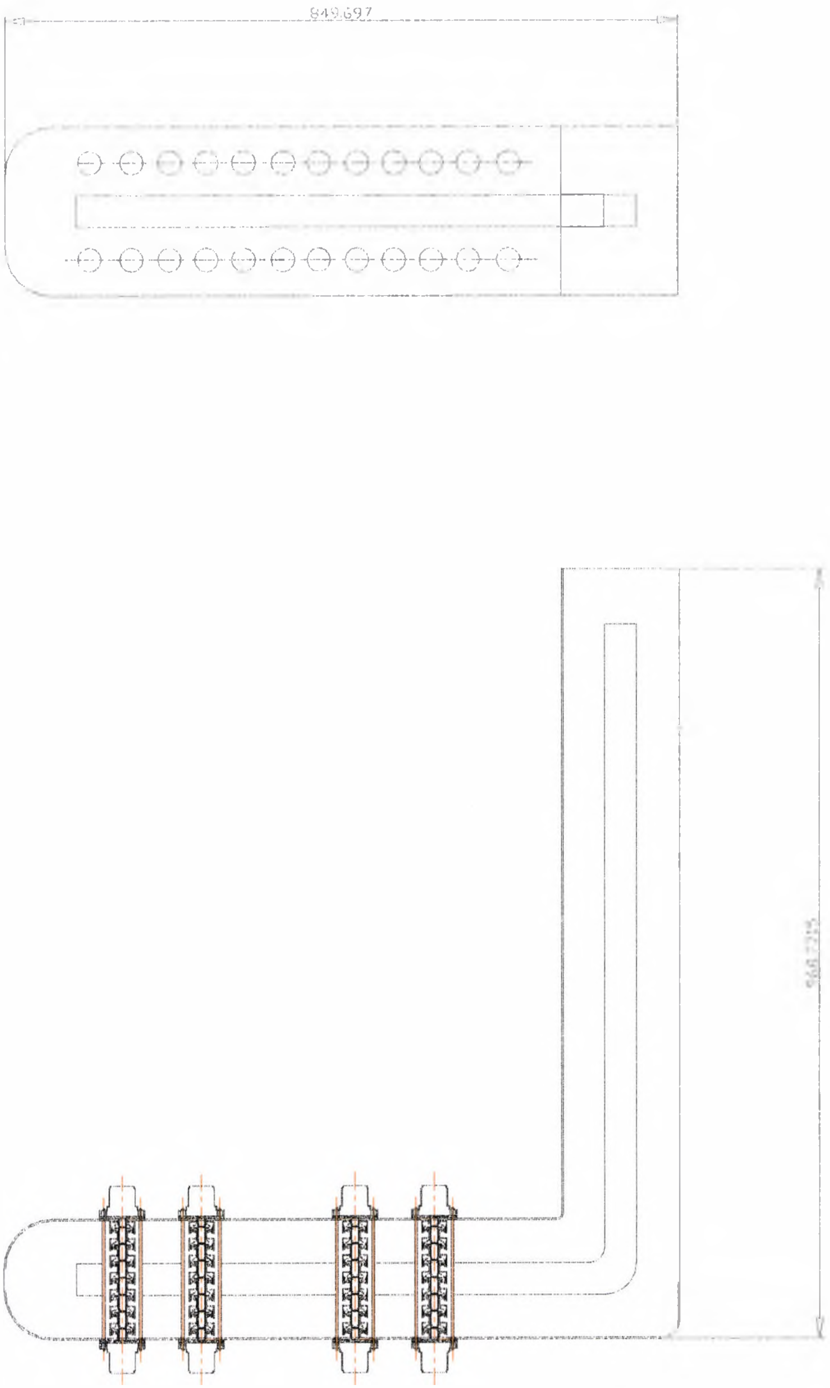

Fig.A-5 Alternative manifold design.

APPENDIX-B Material properties

Electrolyte (Yittra stabilised zirconia)

Melting point [^{o}c]	2680
Density [g/cm^3]	5.90
Ionic conductivity [Ω^{-1}cm^{-1}]	0.12
Thermal conductivity [w/cm•k]	0.02
Thermal expansion coefficient [cm/cm•k]	10.8x10^{-6}
Young's modulus [GPa]	220
Fracture toughness [MN•m $^{-3/2}$]	3
Poisson's ratio	0.32

Cathode ($L_aM_nO_3$)

Melting point [^{o}c]	1880
Density [g/cm^3]	6.57
Electrical conductivity [Ω^{-1}cm^{-1}]	130
Thermal conductivity [w/cm•k]	0.04
Thermal expansion coefficient [cm/cm•k]	11.2x10^{-6}
Young's modulus [GPa]	240
Poisson's ratio	0.25

Anode (Nickel cermet)

Melting point [^{o}c]	1453
Density [g/cm^3]	6.87
Electrical conductivity [Ω^{-1}cm^{-1}]	500
Thermal conductivity [w/cm•k]	1.32
Thermal expansion coefficient [cm/cm•k]	12.5x10^{-6}
Young's modulus [GPa]	231
Poisson's ratio	0.28

Interconnect ($L_aC_rO_3$)

Melting point [^{o}c]	2510
Density [g/cm^3]	6.74
Electrical conductivity [Ω^{-1}cm^{-1}]	14
Thermal conductivity [w/cm•k]	0.04
Thermal expansion coefficient [cm/cm•k]	9.2x10^{-6}
Bending strength [Mpa]	100

Inconnel

Melting point [^{o}c]	1398
Density [g/cm^3]	8.25
Thermal conductivity [w/cm•k]	0.228

Methane

Boiling point [^{o}c]	-434.2
Density [g/cm^3]	0.554
Thermal conductivity [w/cm•k]	0.035
Molecular weight	16.004
Specific heat(c_p)[J/kg•k]	2260

APPENDIX – C Mathematical models

C-1 Electrochemical model

```
SUBROUTINE CALCURRENT ( T,B,C,D,DI,F1,F2,J,L,V,G,I,U,Res,Cur)
c
c=====================
c
c this function returns the current density A/cm**2
c
c solves the electrochemical model
c
c=====================
c-----R - Gas constant[j/mole k]
c----- Far -Faraday constant[col/mol]
c-----Density of methane(ro)[g/m**3]
c-----weight of a single cell(Wt)[kg]
c-----electrolyte cathode and anode resistivity (re,rc & ra)[ohm-cm]

c-----C = electrolyte thickness cm ---max=0.25mm---min = 0.1mm
c-----electrode thickness---max=0.03mm---min=0.01
c-----F1= ANODE THICKNESS
c-----F2= CATHODE THICHNESS
c-----T= OPERATING TEMP KELVIN, USUALLY 1273
c-----B= INTERCONECT LENGTH, CM
c-----J = fuel flow rate m**3/sec
c-----L= NUMBER OF CELLS IN SERIES ( SAME FUEL FLOW PATH )
c-----I=TOTAL CURRENT = CUR*AREA
c-----all dimensions in cm



       Real J,I
      Pi = 3.14
      re = 9.89
      rc = 0.013
      ra = 0.001
      Far = 96485.3
      R = 8.3145
      ro = 665
      Wt = 0.2
      A = Pi*0.25*(D**2-di**2)
      Pp1 = 0.97
      Theta = ((1/(re*C))*((rc/F1)+(ra/F2)))**0.5
      Res1 = ((rc*ra)/(F1*F2))*(2+(B*Theta*sinh(D*Theta)))
      Res2 = ((rc/F1)**2+(ra/F2)**2)*cosh(D*Theta)
      Res3 = Theta*Pi*((rc/F1)+(ra/F2))*sinh(D*Theta)
      Res = (Res1+Res2)/Res3
      fi=0.0
      AVGCUR=0.0
```

```
      do 66 ki=1,10
         Pp2 = Pp1-0.085
         li = 0
1         xi = abs((Pp1+Pp2)/2)
         li = li+1
c----------oxygen Pp taken constant at 0.21
         Fu = alog((0.458*xi)/(1-xi))
         Er = 0.925+(R*T*Fu)/(2*Far)
         Cur = (Er-V)/Res
         AVGCUR=AVGCUR+Cur
c-----f is the fuel consumption in a node [g/s]
c-----16.043 grams in one mole of methane
         f = ((Cur*16.043*A*0.1)/(2*Far*ro))+fi
c-----Xf is the fuel(H2) fraction left unconsumed
         Xf = (J-f)/J
         if (abs(Pp2-Xf).gt.1.0E-6) then
            Pp2 = Xf
            go to 1
         end if
         if (li.gt.1000) then
            print*,'not converging in 1000 steps'
            stop
         else if (abs(Pp2-Xf).lt.1.0E-6) then
c              print*,'Er=',Er
c              print*,'Pp2=',Pp2
c              print*,' number of iterations =',li
         end if
       fi=f
 66   continue
       AVGCUR=AVGCUR/10.0
       I = AVGCUR*A
       G=100*(1-((J-(f*L))/J))
       U = ((T-800)*(200-F1))/200
        RETURN
        end
```

```
c================
c THIS PROGRAM SEARCHES THE SOLUTION SPACE FOR
c A SOLID OXIDE STACK. IT SOLVES THE ELECTROCHEMICAL MODEL
c FOR A SOFC
c================
c
c SET UP SOME ARRAYS TO REMEMBER THE BEST 100 SOLUTIONS
c
     DIMENSION BCRIT(100),BB(100),BC(100),BD(100)
     DIMENSION BDI(100),BF1(100),BF2(100),BJ(100)
     DIMENSION LB(100),BV(100),BG(100),BI(100),BU(100),NB(100)
     Real J,I,jstart
c
c=========
c   SET BEST CRITERIA TO ALL ZERO
c=========
c
       DO 55 KK=1,100
  55   BCRIT(KK)=0.0
c

       Wt = 0.2
c     print*,'enter value for interconnect length'
c    read*,B
c     print*,'enter value for electrolyte thickness'
c     read*,C
c     print*,'enter cell outer diameter'
c     read*,D
c     print*,'enter cell inner diameter'
c     read*,di
c     print*,'enter cathode thickness'
c     read*,F1
c     print*,'anode thickness'
c     read*,F2
c     print*,'enter rate of fuel flow'
c     read*,J
c     print*,'enter number of cells in a stack'
c     read*,L
c     print*,'enter cell voltage'
c     read*,V
c==========
c set up inital starting values for parameters
c===========
c
     Bstart=3.0
     Cstart=0.01
     DSTART=2.0
     DISTART=1.5
     F1=0.0025
     F2=0.0025
```

```
      Jstart=3.5E-5
      LSTART=5
      V=0.75
      T = 1273
      P = 1.0E3
c
c=========
c whizz around solution space
c changing parameter values
c=========
c
      do 100 jjs=1,5

      j=jstart + (jjs-1)*(jstart*0.1)
      do 100 jjb=1,10
      b=bstart +(jjb-1)*0.5

      do 100 jjc= 1,10
      c=cstart +(jjc-1)*0.001

      DO 100 JJ = 1 ,7
           D=DSTART+((JJ-1))

      DO 100 JJL=1,20
      L=LSTART+JJL
      do 100 jju=1,5
      rjju=jju-1
      DI=DISTART + rjju*0.25

      IF (DI.GT.D) GO TO 100
c
c=========
c calculate current, number of stacks in parallel etc
c=======
c
       CALL CALCURRENT(T,B,C,D,DI,F1,F2,J,L,V,G,I,U,Res,CUR)
      IF (I.LE.0.0)GO TO 100
      IF ( G.GT. 85.0) GO TO 100
      IF (G.LT.70.0) GO TO 100


c
c===========
c G is the % of fuel used - good idea to keep below 80%
c I is the current - can go negative with invalid fuel flows
c===========
c
       N= (2*P/(V*I*L) + 1)/2

c
c=============
```

```
c estimate amount of material in electrolyte, plus electrodes
c=============
c
      WT=(( 3.14159*((D/2)**2-(DI/2)**2))*(F1+F2+C))*N*L
c
c============
c ESTIMATE TOTAL VOLUME OF ONE CELL, AS INTERCONNECT
LENGTH
c TIMES AREA
c
c============
c
      CELLVOL= ((D/2)**2)*3.14159*B
c
c=============
c ESTIMATE CELL START UP TIMES , AS THERMAL STRESSES
INCREASE
c WITH CELL SURFACE AREA
c
c=============
c
      STIME=(D*D)
c
c==============
c CALCULATE VOLUME AS TWICE TOTAL VOLUME OF CELLS
c==============
c
      TOTVOL= CELLVOL*L*N*2
c
c===========
c CALCULATE OPTIMISATION CRITERION
c AS POWER*(FUEL UTILISATION)/(CELLVOLUME * WEIGHT *
STARTUPTIME)
c divide by the internal resistance of the cell times current squared
c TOTAL INTERNAL ELECTRICAL LOSSES INCREASE WITH CELLS IN
SERIES
c=========
c
      CRIT=1000.0*P*G/(TOTVOL*WT*STIME*I*I*RES*L)
c
c=============
c SEE IF THIS DESIGN QUALIFIES FOR AN ENTRY
c IN THE HALL OF FAME
c=============
c
      DO 200 KIL = 1,100,1
      IF(BCRIT(KIL).GT.CRIT) GO TO 200
      IF (BCRIT(KIL).EQ.0.0) GO TO 400
c
c==============
```

```
c SAVE THIS ENTRY - SHUFFLE ALL THE OTHERS DOWN ONE AND
FORGET
c LAST ENTRY
c==============
c

      DO 300 KI4= 99,KIL,-1
      KI3=KI4+1
      BCRIT(KI3)=BCRIT(KI4)
      BB(KI3)= BB(KI4)
      BC(KI3)=BC(KI4)
      BD(KI3)=BD(KI4)
      BDI(KI3)=BDI(KI4)
      BF1(KI3)=BF1(KI4)
      BF2(KI3)=BF2(KI4)
      BJ(KI3)=BJ(KI4)
      LB(KI3)=LB(KI4)
      BV(KI3)=BV(KI4)
      BG(KI3)=BG(KI4)
      BI(KI3)=BI(KI4)
      BU(KI3)=BU(KI4)
 300  NB(KI3)=NB(KI4)

c==========
c SAVE THIS ENTRY
c==========
  400  BCRIT(KIL)=CRIT
      BB(KIL)= B
      BC(KIL)=C
      BD(KIL)=D
      BDI(KIL)=DI
      BF1(KIL)=F1
      BF2(KIL)=F2
      BJ(KIL)=J
      LB(KIL)= L
      BV(KIL)=V
      BG(KIL)=G
      BI(KIL)=I
      BU(KIL)=U
      NB(KIL)=N
      GO TO 100
200 CONTINUE
c
c   NEXT LOOP
c




c======
```

```
c  open data file for results
c======

   open(unit=7, file=’sam.dat’)
   WRITE (7,1000) P,T
1000 FORMAT (1X, ‘POWER=’, F10.2,’ WATTS’, ‘TEMPERATURE=’,
      1F10.2, ‘KELVIN’)
     WRITE (7,1002)
1002 FORMAT (1X, ‘CRITERION    IC     ET     O.DIA   I.DIA      CT
   &      AT    FUEL F.R.  SERIES    V     G%         I
   &           U  PARALLEL’)
    DO 700 M=1,100
     WRITE (7,1001) BCRIT(M),BB(M),BC(M),BD(M),BDI(M),BF1(M),
   1BF2(M),BJ(M),LB(M),BV(M),BG(M),BI(M),BU(M),NB(M)
 700  CONTINUE
    STOP
 1001 FORMAT (1X,2(F10.5,1X,F6.2),1X,F6.2,2(1X,F10.5),
   & F10.7,I8,1x,F4.2,3(1X,F10.5),I8)

         end
```

C-2 CFD- COMMAND FILE

```
>>CFXF3D
 >>OPTIONS
  TWO DIMENSIONS
  BODY FITTED GRID
  TURBULENT FLOW
  INCOMPRESSIBLE FLOW
  USER SCALAR EQUATIONS 3
  END
 >>VARIABLE NAMES
  USER SCALAR1 'X SHEAR STRESS'
  USER SCALAR2 'Y SHEAR STRESS'
  USER SCALAR3 'YPLUS'
>>MODEL TOPOLOGY
 >>INPUT TOPOLOGY
  READ GEOMETRY FILE
>>MODEL DATA
 >>TITLE
  PROBLEM TITLE 'Fuel cell'
 >>PHYSICAL PROPERTIES
  >>STANDARD FLUID
   FLUID 'AIR'
   STANDARD FLUID REFERENCE TEMPERATURE 2.8800E+02
  >>FLUID PARAMETERS
   VISCOSITY 1.783E-05
   DENSITY 1.2256E+00
 >>DIFFERENCING SCHEME
  U VELOCITY 'HIGHER UPWIND'
  V VELOCITY 'HIGHER UPWIND'
>>SOLVER DATA
 >>PROGRAM CONTROL
  MAXIMUM NUMBER OF ITERATIONS 60
  MASS SOURCE TOLERANCE 1.0E-6
>>MODEL BOUNDARY CONDITIONS
 >>SET VARIABLES
  PATCH NAME 'IN'
  V VELOCITY 2.00
 >>SET VARIABLES
  PATCH NAME 'OUT'
  PRESSURE 0.0
>>OUTPUT OPTIONS
 >>FRONTEND PRINTING
  NO FRONTEND PRINTING
>>STOP
```