

# **Assessing scalability and economic viability of a membraneless divergent electrode flow-through electrolyser through design modifications**

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## ABSTRACT

The alkaline Divergent-Electrode-Flow-Through (DEFT™) electrolyser represents the core novelty of the presented technology in that it utilises the flow of electrolyte entering an electrode gap with the subsequent diversion of fluid through porous electrodes to maintain separation of the produced hydrogen and oxygen gases. Inventiveness is introduced by the absence of a conventional ion-exchange membrane or diaphragm, and consequently, none of the limitations associated with this component are present. The core advantages of the technology are defined by (i) A simplified reactor design with fewer components reducing capital, operation and maintenance costs, (ii) Temperature limitations are defined only by the materials of construction, with potential to operate at intermediate temperatures (150 – 300°C), (iii) Greater operating current densities thresholds in contrast to conventional alkaline systems with the ability to easily accept a fluctuating load, ideally from a renewable energy source, and (iv) Reduced cell resistance through effective bubble management and removal of membrane/diaphragm resistances.

Early-stage prototype developments showed high current density thresholds and impressive current-voltage (IV) data with  $1.36 \text{ A.cm}^{-2}$  achieved at 2.5 VDC [1]. The technology, however, relied on high electrolytic solution throughput with associated flow velocities of  $0.075 \text{ m.s}^{-1}$  to maintain high purity hydrogen gas production (>99 vol%). This brought about two notable drawbacks as the technology exhibited low system efficiencies (<40 HHV%) due to high parasitic loads and was limited in scaling ability (electrodes size of 30 mm in diameter). The purpose of this study was to address these issues through iterative design modifications. This included the commissioning of a first phase prototype for investigation followed by the design, build and commissioning of a commercial representative 3 – 5 kg/day  $\text{H}_2$  demonstration plant. The objective was to obtain representative performance and economic data such that the economic viability of the technology could be assessed through comparisons to existing electrolytic hydrogen generation solutions. The study culminated into four major design modifications to the original DEFT™ prototype design, these include:

1. The inclusion of a non-conductive mesh (nylon filtration material), which served the purpose of (i) increasing the flux distribution across larger electrode surfaces by providing a source of backpressure and amplifying flow velocities (at set flowrates) into the electrode chamber, and (ii) providing resistance to mass transfer for gas-crossover of larger gas bubbles (with high buoyancy forces).
2. Modifying the electrode to an annulus design such that a flow path can be defined between the outer and inner diameter while still allowing the electrode to be scalable.

3. Modifying the electrolyte injection and bi-phase solution collection manifolds such that backflow and mixing in the electrolyser stack are minimised.
4. Modifying the electrolyser stack to a bipolar configuration allowing for a compact and scalable design that operate with lower amperage power conditioning equipment.

These modifications to the reactor's design/configuration allowed for high purity gas production, >99%, at flow velocities of  $0.0002 \text{ m.s}^{-1}$ , without the use of a conventional diaphragm or membrane resulting in a substantial reduction in parasitic loads and subsequent improvement in system efficiencies. A higher heating value (HHV) efficiency of 60.6% and current density of  $200 \text{ mA.cm}^{-2}$  was achieved at a flow velocity of  $0.0002 \text{ m.s}^{-1}$ , an operating temperature and voltage of  $80^\circ\text{C}$  and 2.0 VDC respectively, utilising pure nickel electrodes with no catalyst coating. This relates to an overall power consumption of  $65 \text{ kWh/kg H}_2$  ( $5.44 \text{ kWh/Nm}^3 \text{ H}_2$ ).

At the high end of the voltage range (2.4 VDC), current densities up to  $400 \text{ mA.cm}^{-2}$  were achieved at operating temperatures of  $80^\circ\text{C}$ , a flowrate of  $45 \text{ L.min}^{-1}$  and operating voltages of  $\pm 2.4 \text{ VDC}$ . Total system energy consumptions ranged between  $64 - 68 \text{ kWh/kg H}_2$  at an operating voltage of  $1.8 - 2.4 \text{ VDC}$  respectively, with hydrogen production rates between  $3 - 5 \text{ kg/day}$  being achieved. Furthermore, the DEFT™  $3 - 5 \text{ kg/day H}_2$  system (the DEFT™ 2.5 unit) was able to successfully lower the parasitic load of the system to  $\sim 2.24 - 13.26 \%$  (previously noted to be as high as  $60 - 80\%$ ) [1] of the total system load by employing lower electrolytic flowrates, while maintaining a safe purity of both oxygen and hydrogen products. At the lower flowrates the DEFT™ unit was able to achieve current densities comparable to industrial standards, but at the expense of a higher energy consumption. While the performance of the system can be increased through the introduction of a catalyst, no significant benefit of operating with enhanced electrolytic flow (compared to the electrolytic flowrate of conventional systems) was observed for the current configuration of the DEFT™ 2.5 unit. DEFT™, however, has the potential to further exploit its membraneless operation through targeting novel operating environments such as the use of unconventional electrolytes, dense electrodes and higher temperature and pressure operation.

Upon the fabrication of the DEFT™ 2.5 unit, a detailed techno-economic analysis was carried out. It was found that a commercial DEFT™ 2.5 unit, employing standard, uncoated, nickel electrodes, operating at similar efficiencies to industrial standards, resulted in Capital costs noted as  $\sim 10.7\%$  higher than the conventional units. The plant can achieve a best-case total production cost of  $6.76 \text{ \$/kg H}_2$  and a CAPEX cost of  $1.51 \text{ \$/kg H}_2$ . With OPEX costs equating to approximately  $0.55 \text{ \$/kg H}_2$ , while electrical costs are  $\sim 4.70 \text{ \$/kg H}_2$ . Studies indicate the costs per  $\text{kg H}_2$  can be improved with scale-up whereby hydrogen costs within the  $5 \text{ \$/kg H}_2$  region can be achieved.

Key terms: Membraneless electrolysis, Alkaline Water Electrolysis, Electrolytic Hydrogen

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## LIST OF SYMBOLS

|               |                                                             |
|---------------|-------------------------------------------------------------|
| $Q$           | Volumetric Flowrate ( $\text{m}^3.\text{hr}^{-1}$ )         |
| $\rho$        | Density ( $\text{kg}/\text{m}^3$ )                          |
| $g$           | Gravitational Constant ( $\text{m}.\text{s}^{-2}$ )         |
| $h$           | Height (m)                                                  |
| $P_s$         | Shaft Power (kW)                                            |
| $\eta_{pump}$ | Pump efficiency                                             |
| $v$           | Velocity ( $\text{m}.\text{s}^{-1}$ )                       |
| $A$           | Geometric Area ( $\text{m}^2$ )                             |
| $E$           | Reduction Potential (V)                                     |
| $H$           | Molar Enthalpy ( $\text{kJ}.\text{mol}^{-1}$ )              |
| $T$           | Absolute Temperature (K)                                    |
| $S$           | Entropy ( $\text{kJ}.\text{mol}^{-1}$ )                     |
| $G$           | Gibbs Free Energy ( $\text{kJ}.\text{mol}^{-1}$ )           |
| $R$           | Gas Constant ( $\text{J}.\text{mol}^{-1}.\text{K}^{-1}$ )   |
| $F$           | Faraday Constant ( $\text{C}.\text{mol}^{-1}$ )             |
| $P$           | Pressure (Pa)                                               |
| $\alpha$      | Activity                                                    |
| $C$           | Heat Capacity ( $\text{J}.\text{K}^{-1}$ )                  |
| $L_v$         | Latent Heat of vaporisation ( $\text{kJ}.\text{mol}^{-1}$ ) |
| $R_X$         | Cell resistance (ohms)                                      |
| $\eta_X$      | Overpotential (V)                                           |
| $j$           | Current density ( $\text{A}.\text{cm}^{-2}$ )               |
| $j_0$         | Exchange current density ( $\text{A}.\text{cm}^{-2}$ )      |

|                 |                                     |
|-----------------|-------------------------------------|
| $I$             | Current (A)                         |
| $\alpha_X$      | Exchange Coefficient                |
| $C_R$           | Concentration (M)                   |
| $k_X$           | Rate Constant                       |
| $\beta$         | Tafel slope (mV)                    |
| $\varepsilon_X$ | Efficiency                          |
| $m_{H_2}$       | Mass flowrate (kg.s <sup>-1</sup> ) |
| $t$             | Time (s)                            |
| $M_X$           | Molar Mass (g.mol <sup>-1</sup> )   |

## NOMENCLATURE

|         |                                           |
|---------|-------------------------------------------|
| SMR     | Steam Methane Reforming                   |
| US      | United States                             |
| DoE     | Department of Energy                      |
| FCEV    | Fuel Cell Electric Vehicle                |
| CCUS    | Carbon Capture, Utilisation and Storage   |
| CAPEX   | Capital Expenditure                       |
| OPEX    | Operational Expenditure                   |
| O&M     | Operation and Maintenance                 |
| HHV     | Higher Heating Value                      |
| LHV     | Lower Heating Value                       |
| NREL    | National Renewable Energy Laboratory      |
| IEA     | International Energy Agency               |
| PGM     | Platinum Group Metals                     |
| DEFT    | Divergent Electrode Flow Through          |
| MCE     | Multiple Circular Electrode               |
| CFD     | Computational Fluid Dynamics              |
| HFP     | Horizontal Filter Press                   |
| MCFP    | Mono-Circular Filter Press                |
| Bi-MCFP | Dual injection Mono-Circular Filter Press |
| ICE     | International Conference of Electrolysis  |
| HAZOP   | Hazard and Operability Study              |
| AWE     | Alkaline Water Electrolysis               |
| PEME    | Proton Exchange Membrane Electrolysis     |
| AEM     | Alkaline Exchange Membrane                |
| SOE     | Solid Oxide Electrolysis                  |
| MEA     | Membrane Electrode Assembly               |
| OER     | Oxygen Evolution Reaction                 |
| HER     | Hydrogen Evolution Reaction               |

|       |                                            |
|-------|--------------------------------------------|
| HEL   | Higher Explosive Limit                     |
| LEL   | Lower Explosive Limit                      |
| SHE   | Standard Hydrogen Electrode                |
| PPS   | Polyphenylene sulphide                     |
| PFSA  | Perfluoro-sulfonic acid                    |
| PV    | Photovoltaic                               |
| BOP   | Balance of Plant                           |
| IRENA | International Renewable Energy Agency      |
| PFD   | Process Flow Diagram                       |
| P&ID  | Piping and Instrumentation Diagram         |
| VFD   | Variable Frequency Drive                   |
| PLC   | Programmable Logic Controller              |
| TIA   | Totally Integrated Automation              |
| SCADA | Supervisory control and data acquisition   |
| ASTM  | American Society for Testing and Materials |
| DW    | Dutch Weave                                |
| PW    | Plain Weave                                |
| NS    | Non-Conductive Mesh                        |
| DC    | Direct Current                             |
| AC    | Alternating Current                        |

# CHAPTER 1 - INTRODUCTION

## 1.1 Overview

Hydrogen is one of the most abundant elements in the universe, it has a high heat capacity, has one of the highest energy densities by mass and is a building block of organic matter and many other fuels and industrial chemicals on which the world relies on [2]. Consequently, industry has found many uses for hydrogen, which include its use as an industrial feedstock, as an energy carrier and coolant to name a few [3]. Hydrogen is abundant on earth, however, it is found strongly bonded to oxygen to form water. Extracting hydrogen from water through electrolysis using renewable energy could serve as a means to decarbonise many of the industries that contribute to climate change.

Beyond hydrogen's industrial uses, it has gained much interest due to the potential role it could play in the renewable energy market. Renewable energy sources, which include wind, solar, hydro, tidal, and geothermal, provide a substitute for energy production from carbonaceous sources addressing the issues of diminishing fossil fuel reserves and global warming. Most of these modes of clean energy production are unfortunately intermittent, therefore, for renewable energy to re-shape the energy sector, effective energy storage and distribution mechanisms need to be in place. For widespread adoption of renewable energy sources, energy storage methods need to offer flexibility and high storage capacities. For renewable energy to reshape the transportation sector, long haul modes of transportation would require an energy storage mechanism that has a superior power to weight ratio compared to what is offered by existing storage methods such as batteries. Decentralised green hydrogen production is a viable solution as the hydrogen produced (having a higher heating value energy capacity of 39.4 kWh/kg [4]) would allow for high capacity energy storage for renewable energy farms and remote locations, the transportation of renewable energy and onsite rapid fuelling for multiple modes of transportation without greatly reducing payload capacities. Further to this, renewable electrolytic hydrogen provides a pathway to producing carbon-neutral conventional fuels and high energy density liquids as electrolytic hydrogen can be combined with CO<sub>2</sub> extracted from the air or point sources to produce methanol [5], [6] and other fuels through the Fischer Tropsch process [7]–[9].

Widespread adoption of electrolytic hydrogen has, however, been hindered by its high production costs when compared to other energy sources or modes of energy storage. Currently, only 4% [10] of the > 55 million metric tonnes [11] of hydrogen produced annually is produced through electrolysis. Most of the world's hydrogen supply is produced using fossil fuels through the processes of Steam Methane Reforming (SMR) and coal gasification. With low-cost natural gas

as a feedstock in SMR and with the ability to process large quantities of gas, the cost of production of SMR hydrogen in the US falls to as low as US\$ 2/kg H<sub>2</sub>, where the cost to produce electrolytic hydrogen ranges from US\$ 4-7/kg H<sub>2</sub> [12], [13]. These costs, however, are based purely on the cost to produce hydrogen onsite, not including compression, possible transportation, and dispensing. With onsite compression, the dispensed cost for SMR hydrogen increases to around US\$4.5/kg H<sub>2</sub> [14]. The costs above, however, were determined by the Department of Energy (DoE) and are based on onsite production costs. A Korean based study estimated that for distributed hydrogen fuelling stations for fuel cell electric vehicles (FCEV) with centralised SMR hydrogen production including distribution, compression and supplier mark-ups, the dispensed cost of hydrogen derived can increase up to \$20/kg H<sub>2</sub> where favourable economics of US\$16.5 – 18/kg H<sub>2</sub> were estimated for onsite decentralised production of electrolytic hydrogen [13], [15]. The cost breakdowns for SMR, coal gasification and electrolytic hydrogen production reported in literature are not consistent as the ultimate cost figure is sensitive to political, geographical, and economic parameters selected in the study, however, there is agreement that use cases exist where easily accessible, widespread adoption of green hydrogen favours onsite electrolytic production in both economics and logistics. Beyond the complex logistics and high cost associated with the distribution of hydrogen from centralised SMR and coal gasification plants, fossil fuel-based production methods result in the emission of a large quantity of greenhouse gases such as CO<sub>2</sub>. With political and economic forces working to reduce the rate of climate change, these carbonaceous production methods are coming under pressure to reduce emissions by either facing penalties for emissions or being forced to implement carbon capture, utilisation and storage (CCUS) techniques. Both of which work to increase production costs.

For widespread market penetration in various industries, electrolytic methods of hydrogen production do not only need to compete with fossil fuel-derived methods of hydrogen production but rather compete with existing energy sources/storage mechanisms. Looking at the commercial and passenger vehicle industry, the current price per unit energy of hydrogen is still higher than that of petroleum-based fuels, however, it has become the target of many countries to lower this value, to start implementing hydrogen as a viable fuel for the transportation sector. According to an analysis conducted by the California Fuel Cell Partnership, the current price per kg of hydrogen in the United States ranges from US\$12.85 to more than US\$16, however, the average price per kg of hydrogen is approximately US\$13.99. The study states that at a gasoline price of US\$3.50 per gallon, hydrogen would need to be readily available at US\$8/kg H<sub>2</sub> to compete on a cost per mile basis [16].

To reach a price where hydrogen could be deemed as competitive to existing technologies, global targets have been set at attaining a hydrogen production price of \$3/kg by 2030 through

sustainable methods such as electrolysis [13], however, to reach this target further developments and advancement in water electrolysis technologies must be made. The cost to produce hydrogen through electrolysis can be broken up into three segments: initial capital costs (CAPEX), electricity costs (OPEX) and maintenance cost (O&M). Initial CAPEX and electrical OPEX reporting for 90 – 94% of the cost to produce hydrogen [17], [18]. Commercial electrolysis systems operate at an energy consumption of 48 – 65 kWh/kg H<sub>2</sub>, which relates to a higher heating value (HHV) efficiency of 60.6 – 82% [13], [19], [20]. The higher efficiency ranges of 82% HHV are, however, not easily achievable and result in a drastic CAPEX increase. An optimal design point for many systems is found at the energy consumptions within the range of 54 – 60 kWh/kg H<sub>2</sub> [19], [20]. Most electrolysis systems operate from grid electricity and consequently are subjected to costs of main grid power supply. This coupled with the moderate overall conversion efficiency results in the electrical OPEX accounting for up to 62 – 80% of the cost to produce hydrogen in large forecourt systems and 22 – 42% in smaller neighbour scale systems [13], [17], [18]. The NREL, in two reports generated by J. Ivy and G. Saur, provided a cost breakdown for the cost to produce electrolytic hydrogen utilising electrolysis systems in the 10, 100 and 1000 kg/day H<sub>2</sub> production range. The reported data was generated utilising the NREL H2A model analysis. System capital costs used in the study were generated through market surveys and incorporates various types of electrolysis systems [17], [18]. Electrical costs were based on industrial electricity prices published in the 2004 Annual Energy Outlook published by the EIA (U.S Energy Information Agency) [17], [18]. Figure 1-1 provides the average of the values presented in both reports.

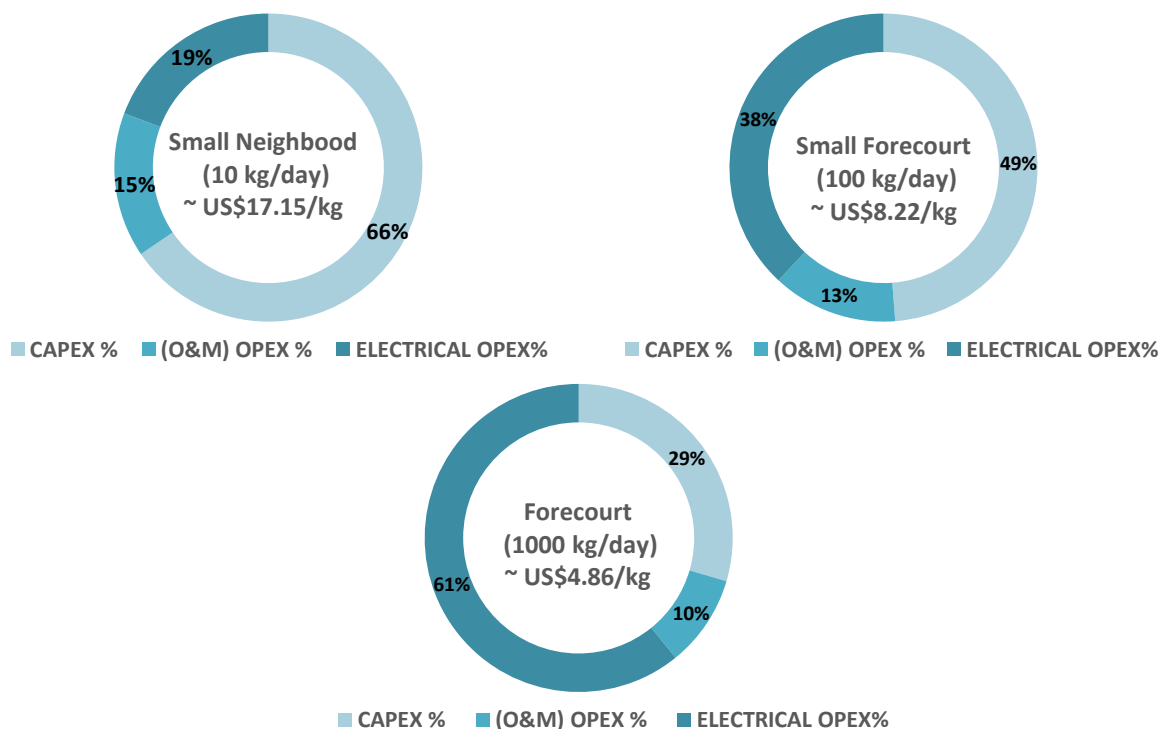


**Figure 1-1: Cost breakdown for electrolytic hydrogen production at various production scales. Adapted from J. Ivy [17] and G. Saur [18]**

Although the cost breakdown is sensitive to a number of parameters such as electrolyser type, system efficiency, cost of electrical input, supplier dependant capital cost, etc., the values provided in Figure 1-1 still provide a representative general overview of the weight various factors carry towards the final cost to produce electrolytic hydrogen. The values in Figure 1-1 are, however, reported for industrial electrical supply from the US grid with a base of 4.85 US\$ cents per kWh [17], [18]. With smaller capacity electrolysis systems, the power capacity input would most likely be too small to allow for industrial grid pricing, thus, it is expected that the electrical weight for the smaller system (<100 kg/day H<sub>2</sub>) would realistically be higher. It is, however, apparent from the data above that to reduce the cost of electrolytic hydrogen production 3 modes of cost reduction would prove most effective, i.e.:

- (i) improve the overall efficiency of the electrolysis system,
- (ii) reduce the CAPEX contribution to production costs, and
- (iii) reduce the cost of electrical inputs to the electrolysis system.

To improve the overall conversation of water electrolysis systems, electrolysers need to be optimised to operate at lower potentials i.e. overpotentials need to be reduced. Waste heat removal, cell resistance, catalytic overpotentials and balance of plant parasitic loads need to be reduced. To reduce the CAPEX contribution to production costs, electrolysis systems need to be simplified and manufactured from low-cost materials thus removing specialised parts, which require complex manufacturing processes or the use of costly platinum group metals (PGM's). Further to this, economies of scale would work to further drive down the CAPEX contribution to production costs. Lastly to reduce the cost of electrical inputs electrolysis systems need to allow for connection to lower-cost energy supply sources such as renewable energy loads. Electrolysers that exhibit characteristics that allow for direct linkage to intermittent/fluctuating loads would be able to capitalise on the ever-reducing cost of renewable power and potentially even work to capture curtailed energy from renewable energy farms.

State-of-the-art electrolysers, for the separation of water into its components, i.e. hydrogen and oxygen, employ a polymer-based membrane to separate the two electrode compartments (cathodic and anodic) to ensure separation of the produced gases. Hydrox Holdings' patented Divergent Electrode Flow-Through (DEFT™) technology [21] rehashes the conventional approach by doing away with polymer-based membrane separators. The DEFT™ technology operates on the principle of manipulating the flow of the electrolytic solution by diverting it through the porous electrodes that result in separation of the produced hydrogen and oxygen gas without the need for a conventional membrane or diaphragm. This simplifies the system and results in

the reduction of both capital and operating expenditure. With their DEFT™ technology, Hydrox Holdings plans to tackle the three areas of cost reduction by aiming to reduce the cost of green hydrogen production without the incorporation of a membrane/diaphragm. The DEFT™ technology, furthermore, has the potential to increase the stack's lifespan, reduce ionic resistances, handle fluctuating currents (making it ideal for renewable energy) and open up the operating parameters and flexibilities of the electrolyser.

The research detailed in this dissertation is based on work conducted at Hydrox Holdings' facility and is a follow-on from the work already published [1], [22]–[24]

## **1.2 Background**

Hydrox Holdings Ltd. was registered in 2002 in South Africa as a public company by a group of businessmen and engineers working on methods to extract hydrogen from water. Activities initially focused on the development of a very basic oxyhydrogen gas generator, which produced a mixture of hydrogen and oxygen gas intending to feed the gas into a modified internal combustion engine. This work continued up to 2012 with activities resulting in the development of a new principle of alkaline water electrolysis that operates on the principle already referred to as Divergent Electrode Flow-Through (DEFT™) alkaline water electrolysis. This technology developed from the need to achieve effective gas separation due to the safety concerns surrounding the generation of explosive hydrogen and oxygen gas mixtures. The DEFT™ operating principle was selected as a means to achieve gas separation while still eliminating the need for a conventional diaphragm/membrane and consequently avoiding the limiting characteristics associated with the use of these structures. Achieving this membraneless approach of water electrolysis would hold the potential of bringing more flexibility to thresholds, operating environments, and operating procedures such as threshold current densities, maximum temperature ratings, electrolyte types, start-up and shut down times, turn down ratios, etc. A basic representation depicting the DEFT™ operating principle approached is provided in Figure 1-2.

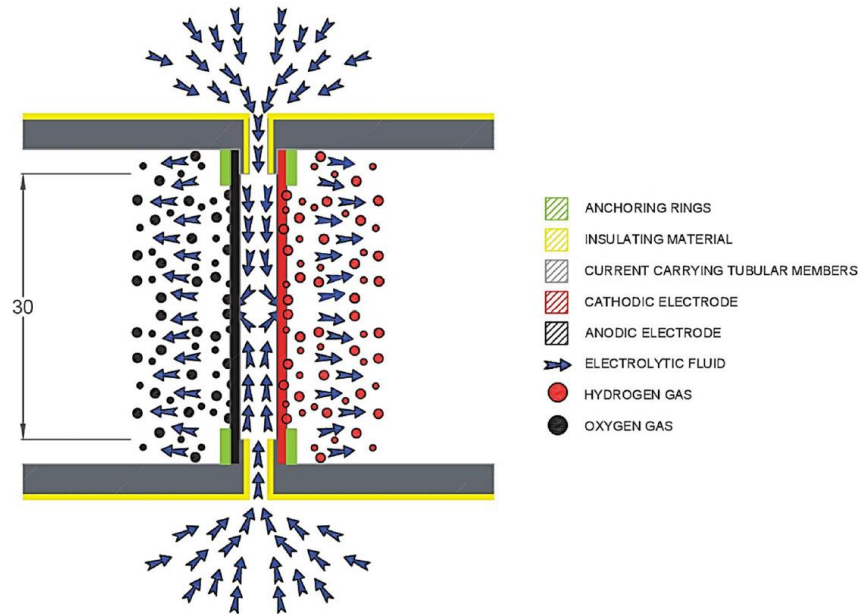


**Figure 1-2: Schematic showing the general DEFT™ operating principle (Extracted from [22])**

### 1.2.1 Early DEFT™ Stack Prototypes

The DEFT™ technology has several similarities to conventional electrolyzers, hence, many key technology principles were adopted from existing alkaline water electrolysis systems. The key differentiating factor of flow-based gas separation, however, presented an area of research that surrounds the investigation of key parameters that affect both electrolyser performance and the extent of gas separation. Variables such as anode and cathode electrode gap, electrolyte conductivity, temperature, electrolytic flowrate, and electrolytic flow path were initially identified as parameters of interest. To investigate the relationship between these parameters, a region of safe and efficient operation needed to be identified as to address early challenges in the development of the technology, several notable test rigs were commissioned and assessed with results having been published in peer-reviewed journals [1], [23], [24]. These test rigs are briefly discussed, as they were instrumental in establishing the baseline of the technology that currently exists.

#### 1.2.1.1 DEFT™ Optimisation Test-Rig

The original DEFT™ test rig was designed with a common pressurised chamber holding 4 pairs of electrodes each having a 30mm diameter active area. Circular electrodes were selected

with the aim of achieving equal electrolytic flow to all electrodes through circumferential flow injection. Figure 1-3 provides a general schematic of the electrode assembly. The rig was constructed and commissioned to investigate the behaviour of the produced gas within the electrode gap and within the interstitial region of the electrodes. Relationships between electrode gap, current density, flow rates and gas purities (indicating extent of gas separation) were investigated. The outcomes of the study are provided in a paper, *“Performance evaluation of a membraneless divergent electrode-flow-through (DEFT) alkaline electrolyser based on optimisation of electrolytic flow and electrode gap”* by Gillespie et al. [24].

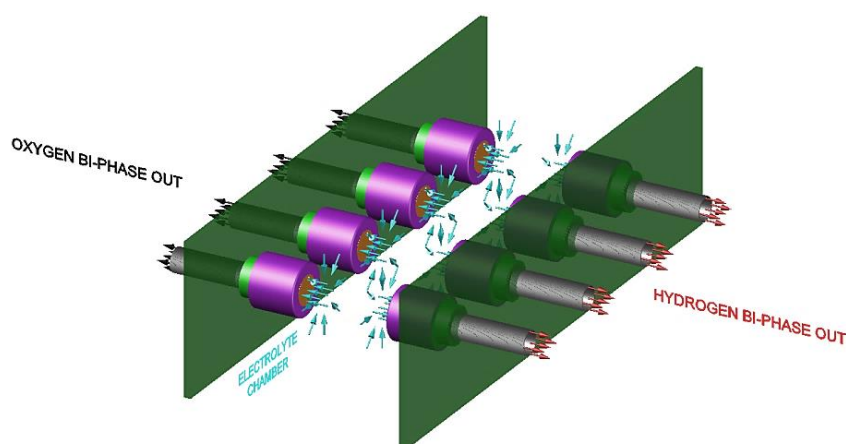


**Figure 1-3: DEFT™ optimisation concept electrode pair arrangement in a pressurised chamber (Extracted from [22])**

This investigation noted that a flow velocity range of  $0.075 - 0.2 \text{ m.s}^{-1}$ , with an electrode gap of 2.5 mm provided an optimal point of operation requiring the lowest electrolytic flow-rate for high purity gas production (+99 vol%). It was noted that as current density increased (through overpotential increases) the required velocity to maintain high gas purities increased. Gas purity data collected at a current density of  $3.5 \text{ A/cm}^2$ , temperature of  $30^\circ\text{C}$  and electrode gap of 2.5mm, provided in Table 1-1, indicated a drop in hydrogen purity at flows below  $0.075 \text{ m.s}^{-1}$  [24].

**Table 1-1: Hydrogen gas purity as a function of electrolytic fluid velocity (Extracted from [24] – Permission Granted in Appendix G)**

| Electrolytic Flow ( $\text{m.s}^{-1}$ ) | Hydrogen purity (vol %) |
|-----------------------------------------|-------------------------|
| 0.2                                     | 99.83                   |
| 0.1                                     | 99.78                   |
| 0.075                                   | 98.98                   |

This drop in gas purity at low flow velocities was believed to have been caused by a large pressure gradient across the front face of the electrodes coupled with the effects of void fraction. This resulted in a “gas meniscus” forming on the front face of both the cathode and anode. The meniscus increased in size until the point at which they converge resulting in cross gas contamination. A representation of this phenomenon is provided in Figure 1-4. Operating at high velocities forces the gas meniscus to the rear of the electrode preventing convergence and hence resulting in improved gas purities [24].

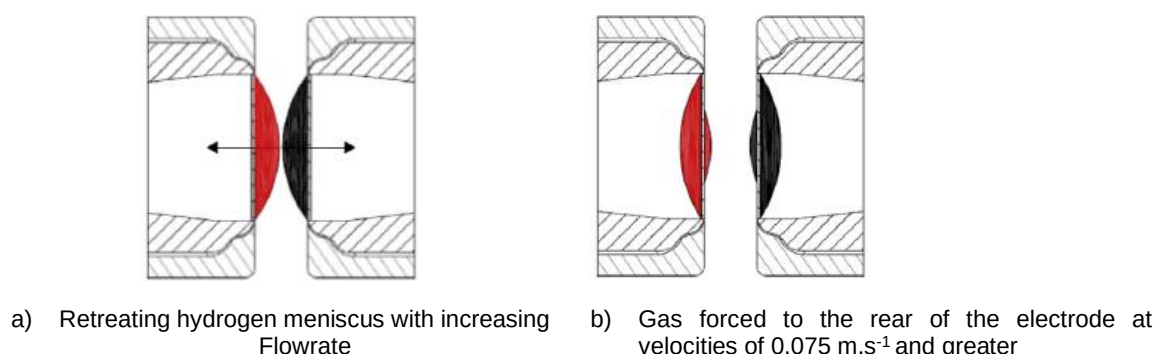


**Figure 1-4: Effects of electrolytic velocity on gas meniscus position**  
(Extracted from [24] – Permission Granted in Appendix G)

### 1.2.1.2 Multiple Circular Electrode (MCE) DEFT™ Reactor

Proceeding from the previous work, and in an early effort to scale the technology, a reactor utilising 49 circular electrode pairs in a common pressurised chamber was designed and commissioned. The electrolytic injection was arranged in a manner that ensured non-preferential flow injection to all electrodes on the periphery of the array, however, it was uncertain whether fluid would be able to penetrate to the centre of the 7x7 array. An image of the electrode array is provided in Figure 1-5. Initial CFD simulation results suggested that it was possible to maintain uniform distribution, however, during experimentation an attempt to maintain equal flux, or even the required flux, though each electrode was not successful. Inadequate gas separation was observed from the cells in the centre of the array resulting in gas entering the electrode gap and ultimately resulting in low gas purities [22]. Further to the issue of low gas purities, the resulting design and number of components involved proved to be a major flaw in the concept, as assembly procedures resulted to be time-consuming and cost-intensive. This design was deemed impractical for commercial development.

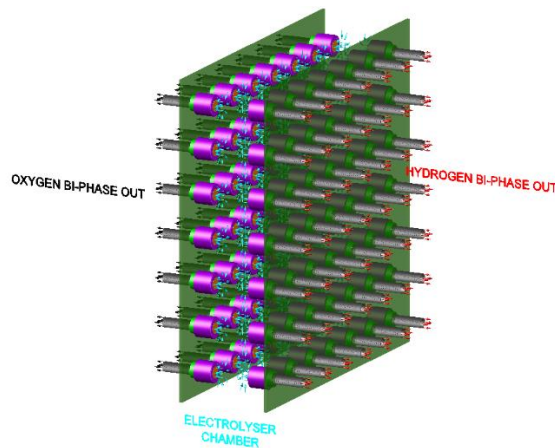


**Figure 1-5: Multiple circular electrode DEFT™ electrode arrangement in a single pressurised chamber (Extracted from [22])**

### 1.2.1.3 Horizontal Filter Press (HFP) DEFT™ Reactor

In an attempt to alter the arrangement methodology of the DEFT™ technology and as a means of exploring alternative methods of technology scale-up, an arrangement utilising elongated rectangular electrodes was fabricated. The design objective for the stack was to allow for the incorporation of high electrode surface areas into a compact volume. Injection of electrolytic solution resultantly would no longer be in a circumferential manner, instead, it would only be from a single side of the rectangular electrode. The idea was to maintain a short and uniform flow path along the electrode to minimise the flux change along the surface of the electrode. Achieving this would allow for the electrode gap to act as a long manifold. Ensuring flow along the length of this manifold would ensure flow is supplied to the entire length of each electrode. Initial CFD results suggested, for a uniform flow velocity/flux distribution to be maintained over this surface, a short flow path would be required and consequently, an optimally deduced flow path of 20 mm was incorporated into the design.

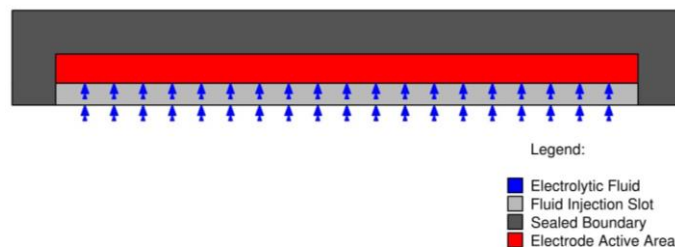


**Figure 1-6: Horizontal filter press DEFT™ reactor arrangement fed from a single slit from a pressurised fluid cavity (Extracted from [23] – Permission Granted in Appendix G)**

Distribution of fluid to the various electrode pairs (4 in total) was assumed to be of the same magnitude, as the 2.5 mm electrode slot provided enough back pressure to equalise pressure

within the fluid introduction cavity. The gas quality obtained from this stack proved to be inadequate, however, it demonstrated an improvement over the MCE reactor [23]. Several rapid prototypes constructed from polycarbonate enabled a view into the inefficient operation of this concept. Gaseous bubbles would accumulate within the electrode gap without being passed through the porous electrodes due to inconsistent flow areas formed on the electrode surface. The design incorporated corners and termination of the fluid path, which would inevitably allow for areas of negligible flow and gas bubble accumulation. This created conditions of cross gas contamination and non-uniform current density distribution [22]. Consequently, the principle of single-sided flow injection to a rectangular electrode was not investigated further. Through this study, however, it was noted that the idea of manifold injection to a single electrode pair allowed for easier flow management when compared to the common sump approach utilised in previous prototypes. The outcomes of the study are provided in a paper, *“Hydrogen production from a rectangular horizontal filter press Divergent Electrode-Flow-Through (DEFT™) alkaline electrolysis stack”* by Gillespie et al [23].

#### **1.2.1.4 Mono-Circular Filter Press (MCFP) DEFT™ Reactor**

The mono-circular filter-press (MCFP) reactor concept was developed as a means of maintaining the improved gas purities associated with circumferential injection to circular electrodes while allowing for manifold electrolytic injection to individual electrode pairs. This particular stack design principle was the most current prototype at the commencement of this study. The design also proved to be the most successful, of the four rapid prototypes designs constructed and tested, to demonstrate safe and efficient stack operation. The arrangement made use of 30 mm circular electrodes whereby each electrode pair is housed in its own independent pressurised chamber and is fed individually with fresh electrolytic fluid through an internal stack injection manifold. Each pair additionally incorporated its own independent gas purge cavity to remove any built-up gas which potentially entered the electrode gap. Each electrode pair, contained within its unique pressurised chamber, was fed directly with fluid from the internal stack manifold. This relieved the issues associated with the large drop in flux across an electrode pair array situated in a common pressurised chamber. A rendering of the general cell design is provided in Figure 1-7.

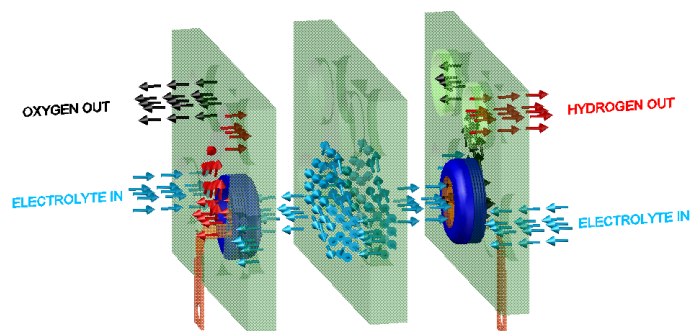


**Figure 1-7: The Mono-Circular Filter-Press (MCFP) DEFT™ stack electrode pair arrangement (Extracted from [1] – Permission Granted in Appendix G)**

The design is unipolar and comprises of 9 major parts, namely: the support plates, housings, and current carriers for both the anode and cathode, a central injection chamber, and the anodic and cathodic electrodes themselves. The design was deemed scalable as the filter press design allowed for enhanced production by incorporating additional electrode pair plates in a parallel configuration to formulate a stack. Hydrogen and oxygen gas purities of 99.81 vol% and 99.5 vol% respectively were achieved at a nominal flow velocity of  $0.075 \text{ m.s}^{-1}$ , while operating at a current density of  $3.5 \text{ A.cm}^{-2}$ . Utilising double  $200 \text{ }\mu\text{m}$  plain nickel Dutch weave electrodes, with no catalytic coating, the stack was able to achieve a current density of  $1.9 \text{ A.cm}^{-2}$  at 2.5 VDC,  $60^\circ\text{C}$  and  $0.075 \text{ m.s}^{-1}$  flow velocity [1]. The stack showed a high level of flexibility with little to no requirement for operational protection philosophies such as down-time protections, ramp-up cycles, etc.

The drawback with this design, however, is the limitation that exists on the electrode diameter. It was noted that increasing the electrode size beyond that of 30 mm (effective flow path of 15 mm) resulted in inadequate flux distribution thus resulting in reduced gas purities. Further to this, the nominal flow velocity of  $0.075 \text{ m.s}^{-1}$  resulted in high electrolytic flowrates, which present a high parasitic load resulting in low overall system efficiencies.

### 1.2.2 Shell GameChanger Project

Together with a publication in the Journal of Power Sources, the study surrounding the MCFP reactor prototype was presented at the International Conference of Electrolysis in 2017 (ICE 2017) in Copenhagen, Denmark. The technology acquired the attention of Shell who invited Hydrox Holdings to apply to the Shell GameChanger program. In 2018 Hydrox Holdings was accepted into the program and was awarded seed funding to embark on the optimisation, design,

fabrication, assembly and testing of a small pre-commercial pilot plant, based on the principle of DEFT™ alkaline electrolysis, that would produce roughly 5 kg/day H<sub>2</sub>.

The project undertaken with Shell GameChanger was intended to showcase DEFT™ electrolysis as a complete system, which involves not only the development of a DEFT™ reactor but the necessary balance of plant and controls required for the safe and effective operation of the system. The project boundary surrounded that of gas generation only, therefore, postproduction gas purification and drying (necessary to reach fuel cell feed purity standards) were not included as part of the scope. This further excluded the need to incorporate compression, storage, and dispensing systems. The outline and scope of the Shell GameChanger project are relevant to this dissertation as all the work presented here was conducted since the commencement of the project. Consequently, methodologies, research design, research scope and dissertation outline were derived within the allowable bounds of the Shell GameChanger project.

The Shell GameChanger project was implemented in three stages, depicted in Figure 1-8, that dealt with the optimisation, design and subsequent, fabrication and testing of a 2.5 Nm<sup>3</sup>/hr H<sub>2</sub> pilot plant.

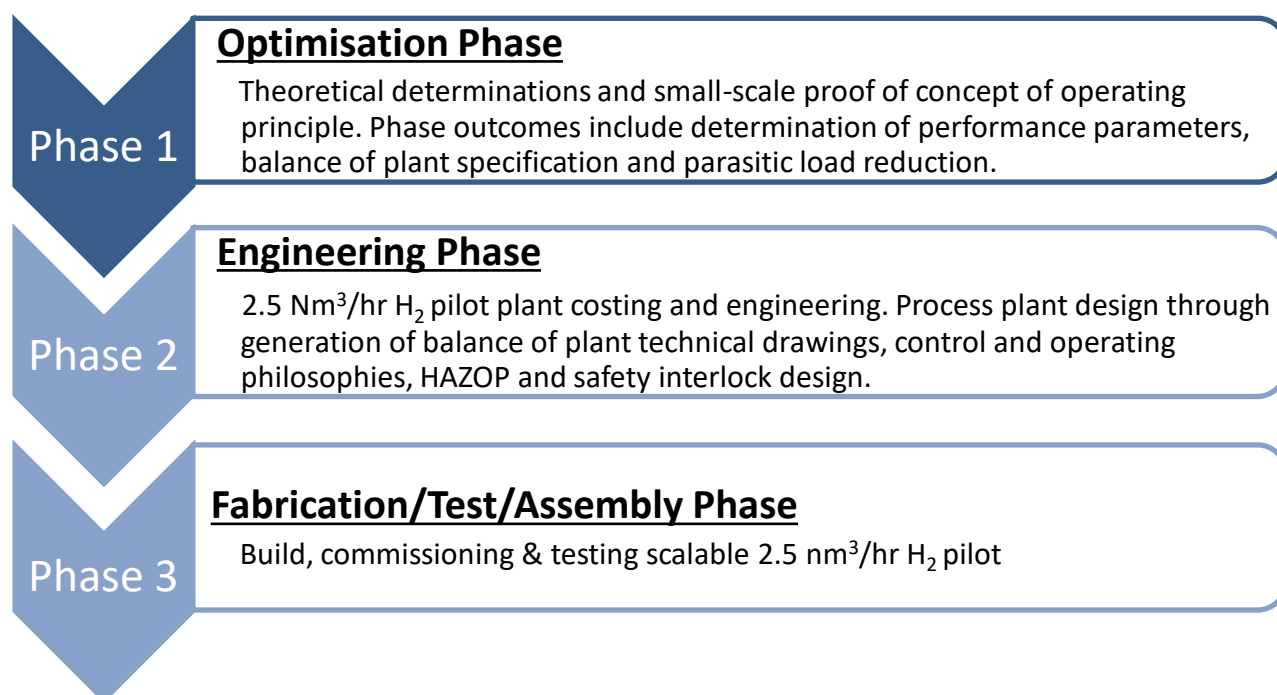


**Figure 1-8: Breakdown of phases outlined in the Shell GameChanger project for the development and assessment of a DEFT™ 2.5 Nm<sup>3</sup>/hr H<sub>2</sub> pilot plant.**

Each phase was subjected to review by internal and external engineers to drive the development along with a strong focus on environmental health and safety and applicable standards. At the commencement of the project the following deliverables/targets were defined:

1. Selection of an optimal mesh configuration to refine stack efficiencies achieved to date. An overall energy consumption target for the system being **< 90 kWh/kg H<sub>2</sub>**.
2. Continuous economic analysis of the initial design outlook of **< 7.5 US\$/kg H<sub>2</sub>** after phase 1, and that of a low CAPEX end design of **< 5 US\$/kg H<sub>2</sub>** after phase 3, based on a small scale production of hydrogen (< 20 kg H<sub>2</sub>/day).
3. An efficient and reliable gas/liquid separation system that yields produced hydrogen and oxygen gases with a continuous gas purity of **> 99.5 vol%**.
4. A stack design refinement that allows for improved scalability.
5. Reduction of plant-parasitic loads to be **< 35%** of the total power consumption of the technology.
6. Identification of the necessary safety interlocks and standards, through a detailed HAZOP study, during the development of the design that complies with the necessary safety standards for the intended demonstrative application.

The study outlined in this dissertation focuses on assessing the scalability and economic viability of a membraneless DEFT™ electrolyser through the identification and further modification of operational and design features that would have a positive effect performance and the ability to scale. This study is therefore not target driven, however, the targets identified within the Shell GameChanger project will be referred to and utilised as “soft targets” for the basis of early-stage assessment and direction.

### **1.3 Problem Statement and Research Motivation**

While the development path of a membraneless DEFT™ electrolyser was mindful to aspects like system efficiencies and engineering practicality, the ideology was to work towards achieving gas separation with only the use of electrolytic flow, while still providing a design that would potentially have the ability to scale, at the expense of high parasitic loads (high pumping loads). Once flow-based gas separation was achieved, system improvements and further product development would commence.

With gas separation having been achieved with the MCFP prototype reactor [1], an assessment of the technology is required to define the technology’s performance and scaling capabilities.

### 1.3.1 Membraneless Electrolysis Motivation

Currently, three main types of water electrolysis technologies are described in detail in the literature, these are alkaline water electrolysis (AWE), proton exchange membrane/polymer electrolyte membrane electrolysis (PEME) and solid oxide electrolysis (SOE) [19], [25]–[29]. SOE technology is less prevalent in the industry due to its specific niche requirements concerning the coupling of the technology to a high heat energy source exceeding 500°C (typically between 700°C and 1000°C) [30]. SOE electrolysis for the moment appears to offer no bulk uptake in the market which resolves in the current market for water electrolysis comprising principally of alkaline and acidic electrolyte technologies of which three foremost configurations exists

- **The gap cells** (evidence of an electrolyte gap between the separator and electrode) – mainly associated with AWE
- **The zero-gap cell** (porous electrodes are pressed against the separator) – mainly associated with AWE
- **The ion-exchange cell** (The solid electrolyte confined to a thin layer, where the layer acts as both the electrolyte and separator) – Associated with PEME and AEM (Anion-exchange membrane) electrolysis.

The above configurations differ in their membrane electrode assembly (MEA); however, they all rely on the function of an internal ion-exchange or porous membrane/diaphragm. The main function of the porous diaphragm/ion-exchange membrane is to keep the produced gases separated; hence, these structures have extremely small pore sizes and complex tortuosity to prevent cross gas contamination. These structures are required to be non-conductive in terms of electron transfer, especially so in zero-gap/advanced alkaline systems, to prevent a direct electrical path between the anode and cathode. As a consequence of this, the materials utilised in the manufacture of these structures results in a low  $\text{OH}^-$  conductivity when compared to that of the electrolyte itself. This is prominent in porous diaphragms as the resistance is a function of the resistivity of the electrolyte and the open area (porosity) of the diaphragm or the amount of electrolyte contained/absorbed within the structure. For example, commercial diaphragm materials at 80°C have a conductivity of  $0.164 \text{ S.cm}^{-1}$  [31] whereas the conductivity of potassium hydroxide electrolyte at the same temperature equates to  $1.38 \text{ S.cm}^{-1}$  [32]. Potassium hydroxide electrolyte, therefore, is roughly 8 times more conductive (8 times less resistant to charge transfer) than separator materials currently utilised in industry. Gas formation within the electrolyte, however, reduces the conductivity of the electrolyte, hence, as current densities increase so does cell resistances. Removing the membrane and hence operating with only electrolyte within the electrode gap would work to reduce cell resistances. Further to this, the DEFT<sup>TM</sup> operating

principle actively provides flow to the electrodes, hence, the gas containing electrolyte is readily removed from the electrode gap maintaining a high electrolyte conductivity. Shear forces, provided by the divergent flow of electrolyte, works to remove bubbles from the surface of the electrode at a rate that is accelerated beyond that of what is experienced under the action of buoyancy forces alone [33].

From this theory, there is the potential that if a small electrode gap is maintained with a low enough parasitic load, a membraneless DEFT™ system could result in favourable system performance, at a reduced capital expenditure. Achieving effective membraneless operation would lay the path for advanced system developments pushing the boundaries of liquid alkaline electrolysis for higher temperature operation, high current density thresholds, effective handling of fluctuating loads and electrolyte variability.

### 1.3.2 Problem Identification

Although membraneless DEFT™ electrolysis can operate at high current densities as a result of the low associated ionic resistance and the drastic associated reduction in resistance associated with bubble generation [34] a certain degree of electrolytic flow needs to be maintained to achieve separation of constituent gases. Assuming operation at  $0.075 \text{ m.s}^{-1}$  with a cell voltage of 2.5 VDC, temperature of  $60^\circ\text{C}$  and resulting current density of roughly  $1\,000 \text{ mA.cm}^2$  [1] the development of a 5 kg/day  $\text{H}_2$  system, requiring a series amperage of 5540 A, a total of  $0.55 \text{ m}^2$  of electrode area would be required and hence a total electrolytic flow-rate of 4 985 L/min. Making use of Eq. 1-1 to determine pump shaft power, at an assumed pump efficiency of 60% and a head of 10 m, a total power rating of 13.57 kW results. This translates to a power consumption of 65.1 kWh/kg  $\text{H}_2$  dedicated to pumping alone [35].

$$P_s = \frac{Q\rho gh}{3.6 \times 10^6 \eta_{\text{pump}}} \quad \text{Eq. 1-1}$$

For DEFT™ to become a viable means of producing low-cost hydrogen, a drastic reduction in the pump power consumption and general system parasitic loads is required. With the target of an overall plant efficiency of  $< 90 \text{ kWh/kg H}_2$  the total parasitic load would be restricted to a value of  $< 31.5 \text{ kWh/kg H}_2$ . The maximum power available for pumping, assuming it to account for 90% of the parasitic load, would thus reduce to  $< 28.35 \text{ kWh/kg H}_2$ . The pump requires a minimum reduction in power consumption by a factor of 3.6 to meet this target. Further reductions in flow

rate would be required to produce a system that would be considered practical for scale-up and provide competitive hydrogen production economics.

The high volumetric flow rates, as a result of operating at a flow velocity of  $0.075 \text{ m.s}^{-1}$ , would not only affect system efficiencies it would also influence the balance of plant setup, from the repercussions associated with the design of liquid processing units to handle high liquid throughputs to the added complexities associated with gas/liquid separation. Although space is largely not a presiding dilemma associated with applications making use of alkaline water electrolysis systems, other process dependant variables are, these include:

- a) Larger process vessels imply greater volumetric quantities of caustic potassium hydroxide that will need to be prepared and disposed of when performing the maintenance of the system.
- b) Larger process vessels imply a greater loss of heat to the environment which would have implications on time to steady-state (efficient operating point), long start-up times would be associated, and once at temperature continuous operation would need to be in place to prevent the system from returning to ambient temperature to prevent further averaged efficiency losses.
- c) The movement of larger volumetric quantities of liquid electrolyte around the system introducing additional pressure head requirements due to additional piping components/manifolds, larger line sizes and complexity in controlling variables associated with level and pressure balancing as a consequence of the high flow.
- d) And where gravitational systems are to be substituted with more advanced means of gas/liquid separation, specialised process vessels such as hollow fibre membrane contactors need to be installed, and hence, the intrinsic process dynamics associated with such systems, such as temperature limitations, need to be considered and accommodated which would add additional complexity to the electrolysis system.

A literary resource reports that with the operation of the MCFP DEFT™ stack it was noted that the flow velocity has a large effect on the resultant current density of the cell. This resolves since at higher flow velocities bubble removal and bubble detachment from the surface of the electrode occurs at an increased rate hence increasing the available surface area for reaction and reducing cell resistances [1], [22]. It is important to note that the amount of energy required to produce electrolytic hydrogen is dependent on the operating potential as well as the selected electrolytic flowrate and pressure head requirement, which ultimately determines the parasitic load. The flowrate required is based on the electrode area and the fluid velocity passing through the porous electrodes, this can be calculated through Eq. 1-2. Where  $Q$  is the volumetric flowrate,  $v$  the

stipulated flow velocity,  $A$  the geometric area of the electrode, and  $n$  the number of electrodes in the stack.

$$Q = vAn \quad \text{Eq. 1-2}$$

The permissible operating fluid velocity is a function of gas purity and is selected to allow for purities >99.5 vol% H<sub>2</sub>. To minimise the overall system energy consumption (kWh/kg H<sub>2</sub>) and hence maximise the overall system efficiency, several variables need to be optimised such as the operating potential (resultant current density), fluid velocity and the number of electrode pairs. All three of these variables are interlinked. Decreasing the fluid velocity results in a current density reduction, therefore, to reach the same production target either the operating potential would need to be increased which affects the stack efficiency or the electrolyser's stack size needs to be increased, which in turn results in an increase in CAPEX and an increase in additional flow and head requirements. An action and consequence diagram depicting this relationship is provided in Figure 1-9.

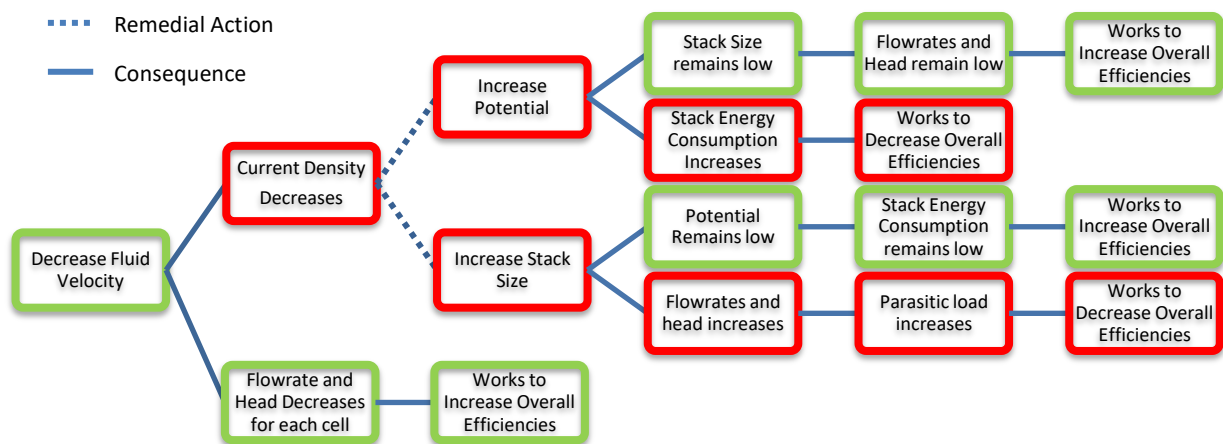


**Figure 1-9: Action and Consequence diagram for changes in operating parameters to a membraneless electrolysis cell**

As Figure 1-9 suggests decreasing the fluid velocity, in an attempt to increase overall efficiencies, decreases the current density which requires remedial action to be taken to reach the same production rate, however, each remedial action taken works to both increase and decrease the overall efficiencies in respect to either increasing or decreasing the parasitic load or the stack power consumption. An investigation needed to be carried out to determine:

- for what combination of these parameters is the overall efficiency maximised,
- would operating at a higher flow velocity ever benefit the overall efficiency,
- to counteract the reduction in current density due to the reduction of flow, what would be the optimal trade-off between increasing stack size (parasitic load) and increasing the operating potential (stack power consumption) to achieve maximum overall efficiencies, and
- are the desired parameters practical? To what extent do you exchange CAPEX and higher efficiencies for increased OPEX and practicality?

As a means of illustrating the relationship between CAPEX (affected by stack size) and OPEX (affected by overall system efficiency), the following flow-based performance scenarios have been generated and are derived from current density data obtained from published current-voltage curves (IV curves) published in literature which relates to MCFP DEFT™ operation with single and double dutch weave Ni200 electrodes [1], [22]. A third performance scenario is examined for the operation of MCFP DEFT™ utilising high-density micro-felt electrodes. The polarisation data is based on data provided by a literary reference utilising a micro-felt substrate of significant available surface area implying a high degree of reactive area with idealistic current densities [36]. A polarisation curve for the three scenarios is provided in Figure 1-10.

The following basis assumptions formed part of this high-level calculation:

- Minimum required average separation flow velocity:  $0.075 \text{ m.s}^{-1}$  [22],
- Solution density at 30% KOH and  $80^{\circ}\text{C}$ :  $1258 \text{ kg.m}^{-3}$  [37],
- MCFP DEFT™ would achieve the same performance data utilising micro-felt electrodes as that reported in literature [36],
- Overall shaft efficiency of pumping: 50%,
- Pressure head to be held constant at 1 Bar head.
- Electrode size equating to 300 mm.

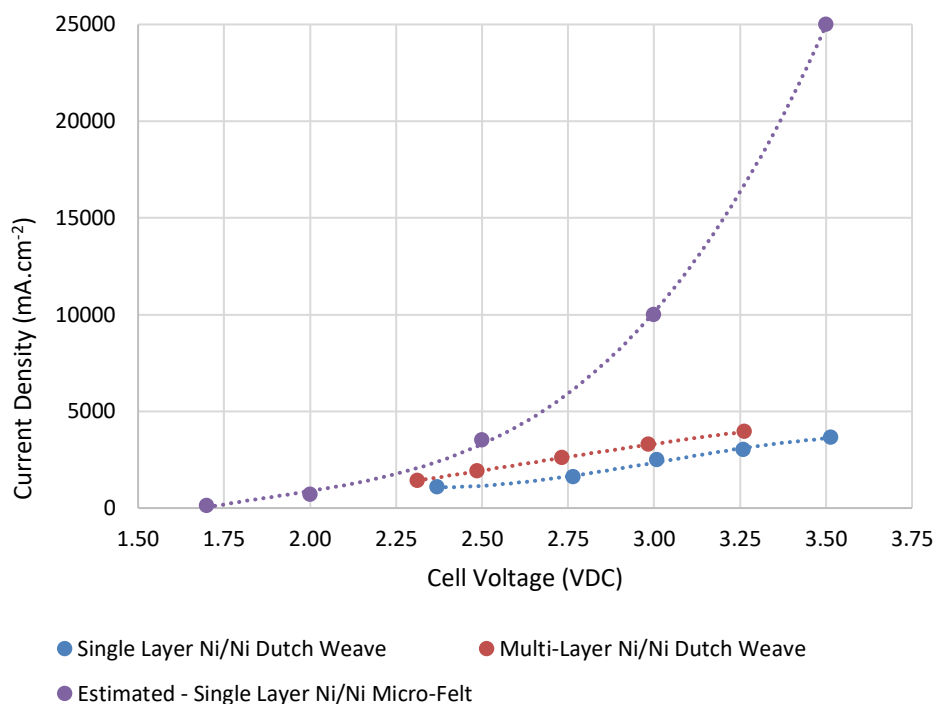
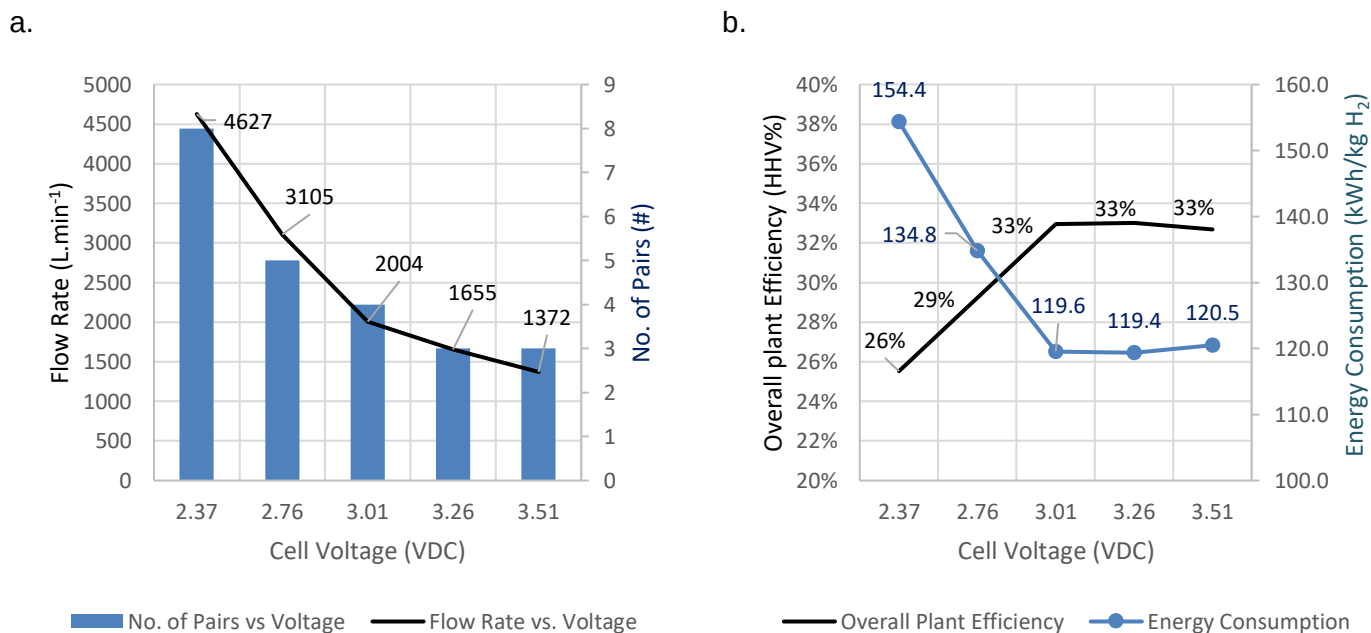


**Figure 1-10: Polarisation curves indicating the basis of the flow-based performance analysis for DEFT™ membraneless electrolysis (Data extracted from [1], [36])**

From the polarisation data provided in Figure 1-10, the determination of the required flowrate was made for each of the performance IV curves represented above



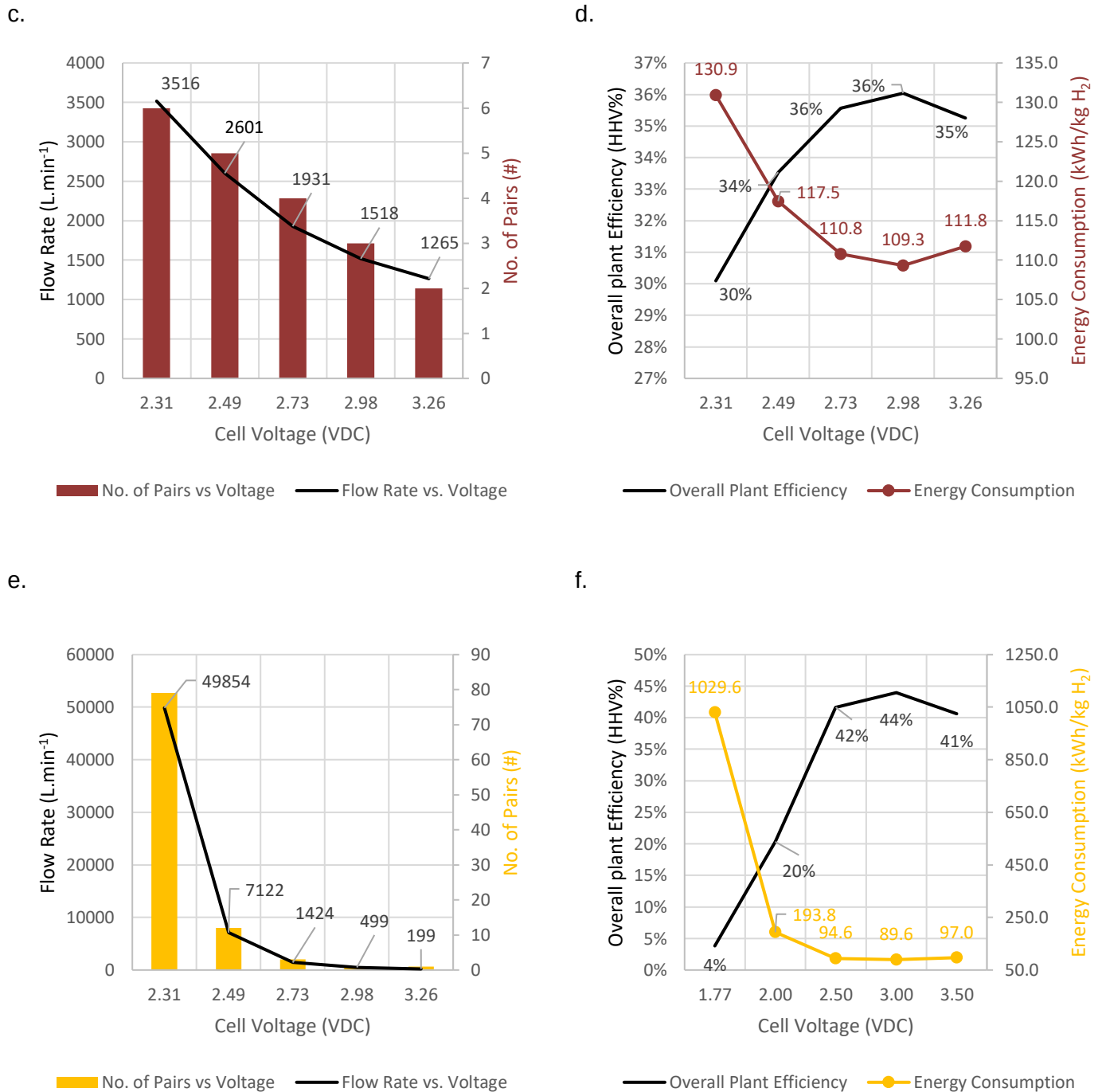


**Figure 1-11: Polarisation (a.) – Total flow rate and No. of electrode pairs of Single layer Ni/Ni dutch weave, (b.) – Overall plant HHV% efficiency and energy consumption of Single layer Ni/Ni dutch weave, (c.) – Total flow rate and No. of electrode pairs of Multi-layer Ni/Ni dutch weave, (d.) – Overall plant HHV% efficiency and energy consumption of multi-layer Ni/Ni dutch weave, (e.) Total flow rate and No. of electrode pairs of Single layer Ni/Ni micro-felt electrodes, (h.) – Overall plant HHV% efficiency and energy consumption of Single layer Ni/Ni micro-felt electrodes**

Upon analysis of curves provided in Figure 1-11 a,b,c,d,e and f, the overall theoretical energy consumption attainable for membraneless DEFT™ resolved to values over 90 kWh/kg H<sub>2</sub>. Further analysis of the curves demonstrates significant solution flows, only reducing to manageable flowrates at high stack operating cell potentials (low stack efficiencies). A constant optimisation between the demand for pumping, separation system complexity and stack operating efficiency is presented. It is notable that with these cases, overall plant efficiency is only minimal for cell potentials above 2.5 VDC. There are, however, no literary record of commercial electrolyzers operating at this cell potential due to implications to overall plant efficiency which is key due to the large weighting of OPEX towards the overall cost to produce hydrogen [38].

Conversely, for circumstances where the energy input cost provided is sufficiently low, such as in the case of low-cost renewable energy inputs, nuclear inputs or operating off curtailed loads, the electrical OPEX cost contribution could diminish to such an extent that CAPEX contributions govern the overall cost to produce electrolytic hydrogen. In such cases, a trade-off of lower CAPEX for higher OPEX may be warranted [36]. It is; however, worth noting that in cases such as curtailed energy hydrogen production only a set quantity of energy will be available during a set time window, hence, the system operating at the higher efficiency would result in the greater quantity of hydrogen produced thus offsetting the CAPEX contribution (\$/kg H<sub>2</sub>) by a larger extent. Similar to the parabolic curves display in Figure 1-11 (energy consumption/energy efficiencies curves), the overall cost to produce hydrogen, assuming negligible energy input costs, would form a parabolic curve on a voltage axis with the inflection point (the lowest cost to produce hydrogen) shifting to lower costs with increasing system efficacies, decreased CAPEX costs and increasing current densities at set overpotentials. This suggests that even in a case of negligible cost of power input, the overall cost to produce hydrogen would still be heavily dependent on system efficiency. Consequently, in both cases of negligible and appreciable energy input cost, it is a necessity to minimise the systems overall power consumption.

Two scenarios, therefore, present themselves as a means of progressing with membraneless DEFT™ electrolysis:

1. Continuation of DEFT™ in a form that would still allow for high flow operation in a pure membraneless configuration but attempt to alter the configuration and electrode structure as to maximise current density and thus minimising the required flow rate through minimising the required electrode as opposed to focussing on efforts to reduce flow velocities. This method represents a costly and time-intensive exercise to investigate several variable dependencies which to date has only been investigated on a high-level basis due to available manpower and funding.

2. Continuation of DEFT™ in a form that incorporates porous materials which makes use of basic filter materials with stipulated aperture sizes to improve flux distributions and reduce required flow velocities. This would enable the drastic reduction in the necessary electrolytic flows with the implication being a reduction in current densities at set cell potentials due to reduced bubble removal and hence higher electrode coverage and electrolyte resistance. The configuration of the stack and balance of plant would start to emulate that of conventional alkaline systems with the difference being that the stack remains largely simplistic and void of the limitations associated with operating with a conventional diaphragm or ion-exchange membrane. This method demonstrated potential within Phase 1 is planned for investigation within phase 1.

#### **1.4 Research Aim and Objectives**

This study aims to assess the scalability and economic viability of a membraneless DEFT™ electrolyser through design modifications. To elaborate further, the aim is to assess the economic viability of the DEFT™ membraneless electrolyser by working to reduce the overall parasitic load of the system and assess the knock-on effects on stack performance, such that a market comparative study can be performed. A secondary aim is to investigate the scaling potential, through assessment, design modification and study. Consequently, investigating a means to increase the effective electrolytic flow path of the electrode, thus increasing the overall electrode area beyond that of 15 mm as detailed in Section 1.2.1.4, allowing for hydrogen production in the kg/day range to be attained.

The objectives of this study are as follows:

1. Identify all relevant bottlenecks that would limit the scaling of the DEFT™ system and determine system parameters that work to reduce system efficiencies.
2. Implement design modifications to tackle the associated bottlenecks through refinements to DEFT™'s electrode assembly and injection chamber to increase electrode size and reduce the flow required for effective gaseous separation.
3. Build, assemble, and commission an early-stage demonstration electrolyser prototype and suitable balance of plant test rig to carry out early proof of concept tests to identify all relevant adjustable parameters affecting system/production efficiencies.
4. Investigate the fluid dynamics associated with various fluid injection configurations, along with the presence and absence of porous layers (electrodes and non-conductive mesh) in the reactor with the aid of Computational Fluid Dynamics (CFD) software.

5. From the early prototype assessment and the CFD results provide a finalised design and configuration for the build of a 3 – 5 kg/day H<sub>2</sub> commercial representative demonstration prototype.
6. Build, assemble, and commission the 3 – 5 kg/day H<sub>2</sub> electrolyser stack and associated plant auxiliaries that provide a representative commercial operation.
7. Ultimately assess scalability, performance, and economic viability of the DEFT™ concept through experimentation and study of the 3 – 5 kg/day H<sub>2</sub> demonstration rig.

## 1.5 Dissertation Outline

This dissertation is presented in a total of 7 chapters, of which, follow a similar phased structure to that defined by the Shell GameChanger project provided in Figure 1-8. This structure allowed for iterative and rapid testing of design modifications and configuration changes in an early small-scale demonstration pilot. From the findings within phase 1, a finalised design for the build of the 3 – 5 kg/day H<sub>2</sub> plant could be established such that the data obtained from its operation would be representative of a commercial electrolysis system.

**Chapter 1** – Background to Shell GameChanger project and a brief introduction to the dynamics of the Hydrogen economy. A brief background into the membraneless DEFT™ technology is provided. The motivation for the technology is established as well as a problem statement defining the requirement for the commencement of this study.

**Chapter 2** – Literature review, which provides the fundamentals of electrolytic hydrogen production. Special attention is given to thermodynamics and sources of overpotentials due to the energy conversion nature of the technology and the associated need to maximise efficiencies of these conversions and secondly, due to the technology's future potential to operate at higher temperatures. Comparisons to existing technologies are provided to establish performance benchmarks. Cell configurations are discussed to provide the necessary background information needed for the successful development for a liquid alkaline stack. Alternative membraneless technologies are investigated. A literature review is provided for catalyst incorporation for the alkaline space. This indicates what performance improvements would be possible if catalyst coatings are to be incorporated into the technology. Lastly, a market review is provided to established techno-economic benchmarks for this assessment.

**Chapter 3** – Commissioning and experimentation work surrounding design and configuration modifications to the original MCFP stack. This included the testing of alternative electrode types

and configurations as well as investigating the flow requirements with the incorporation of non-conductive mesh types. Gas purities and IV data provided the necessary performance indicators.

**Chapter 4** – CFD simulations focusing on investigating the effect of manifold design and associated electrolyte injection into the electrolyser stack on the extent of uniformity of flow distribution amongst the electrode pairs.

**Chapter 5** – Commissioning and testing of the 3 -5 kg/day H<sub>2</sub> commercial demonstration pilot plant. This chapter focuses on performance data generation and assessment. The effect of flow velocities and, temperature on gas purities and current densities formed the basis of this study.

**Chapter 6** – A Techno-economic study was carried out incorporating the data generated in Chapter 5. The OPEX vs CAPEX relationship was investigated for different operating points, and the CAPEX and OPEX data points were compared to industrial benchmarks. Further to this, the effects of economies of scale on these parameters were assessed. Lastly, the cost to produce electrolytic hydrogen was determined for a variety of conditions using the data obtained from the 3 -5 kg/day H<sub>2</sub> commercial demonstration pilot as a basis.

**Chapter 7** – Final research conclusions and future recommendations

## **1.6 Intellectual Property Rights and Colleague Participation**

All intellectual property concerned with the research, design and operating principle of the Hydrox Holdings Ltd. alkaline water electrolyser will remain with the owner. The DEFT™ is patent protected as per WIPO patent WO2013118104A1 [21]. The purpose of this investigation is to assess the scalability and economic viability. In order to do so, modifications to the current MCFP design are required.

As noted, the work detailed in the body of this dissertation was carried out as a project for the company Hydrox Holdings Ltd. situated in Johannesburg, South Africa. The project commenced in 2018 with a team of two engineers, my colleague Malcolm Gillespie and myself Jason Cuomo, working on the project. At the beginning of the year 2020, the team expanded to three engineers with the addition of my colleague Sanusha Govender. As a small team, we worked together and all had a hand in the various aspects of design work to data generation. Although this dissertation has been prepared by myself, many of the aspects in the project were completed with the active input from both of my colleagues. The areas in which my colleagues worked alongside myself and were actively involved were as follows:

**Malcolm Gillespie:**

- Design, fabrication and 3D modelling of the Bi-MCFP electrolyser,
- Commissioning, testing and data generation from the Bi-MCFP pilot plant,
- Design and 3D modelling of the Bipolar Bi-MCFP electrolyser stack,
- Generation of the control and operating procedures and the creation of the associated P&ID diagram,
- Fabrication and procurement of items for the Bipolar Bi-MCFP pilot plant,
- Commissioning and wiring of the Bipolar Bi-MCFP,
- Testing and data generation for the Bipolar Bi-MCFP pilot plant.

**Sanusha Govender:**

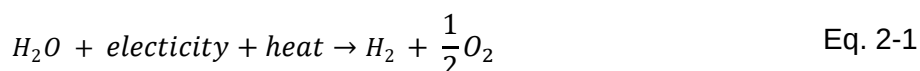
- Commissioning and wiring of the Bipolar Bi-MCFP,
- Testing and data generation for the Bipolar Bi-MCFP pilot plant,
- Market research and generation of costing data for the Bipolar Bi-MCFP pilot plant.

Permission, provided in Appendix G, has been granted by both of my colleagues (Malcolm Gillespie and Sanusha Govender) to publish the data and resources contained in this dissertation. Information of which they play an active role in generating.

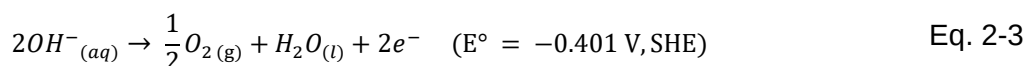
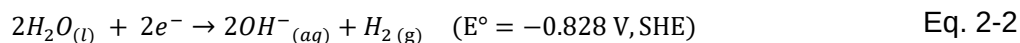
## CHAPTER 2 - LITERATURE REVIEW

### 2.1 Fundamentals of Water Electrolysis

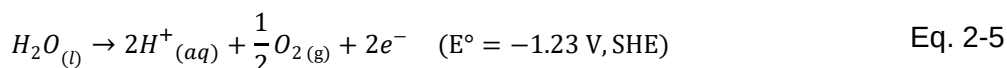
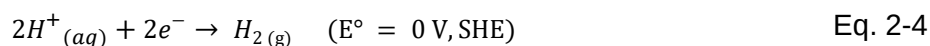
In the process of water electrolysis energy is added in the form of heat and electricity to encourage the dissociation of water into its constituent hydrogen (H<sub>2</sub>) and oxygen (O<sub>2</sub>) gases, as per Eq. 2-1 [39].



The overall electrolytic process involves two half-reactions, a cathodic and anodic redox reaction, known as the hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER) respectively [40]. The HER and OER reactions are dependent on the electrolyte used, hence, the ionic agents in the cell. The three core electrolyte environments are alkaline (OH<sup>-</sup>), acidic (H<sup>+</sup>) and solid oxide (O<sup>2-</sup>). Further to this, the electrolyte can exist as an aqueous solution or as an ion-exchange polymeric or ceramic membrane [24]. The electrolytic production of hydrogen in alkaline media involves the reduction of water molecules to produce hydrogen gas (HER) and the oxidation of hydroxide ions to produce oxygen (OER) [41].



In acidic media, water is oxidised at the anode to form oxygen gas (OER) and proton ions are reduced at the cathode to form hydrogen gas (HER) [41] [42].



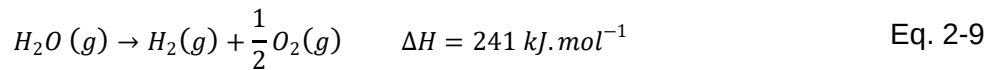
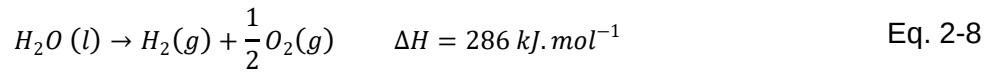
In the case of a solid oxide, water is reduced at the cathode to form hydrogen (HER) and O<sup>2-</sup> ions are conducted through the solid oxide electrolyte to oxidise at the anode forming oxygen gas (OER) [43].





Although the utilisation of different electrolytes results in different reaction pathways the overall reaction is that of Eq. 2-1, and hence, the various operating principles are subjected to the same thermodynamic constraints. Consequently, theories surrounding water electrolysis can be assessed irrespective of the electrochemical cell's operating environment. These fundamental theories of water electrolysis for hydrogen production can, therefore, be broken down into three common areas, i.e. kinetics, thermodynamics, and electrical resistance effects.

### 2.1.1 Thermodynamics



The enthalpy change (heat of reaction) for the formation of hydrogen and oxygen from liquid water equates to 285.8 kJ.mol<sup>-1</sup> at 298 K. This equates to 39.4 kWh/kg H<sub>2</sub> and is known as the higher heating value (HHV) of water [4]. Formation of these product gases from gaseous water (steam) results in an enthalpy change that equates to 241.8 kJ.mol<sup>-1</sup> at 298 K [38][44]. This equates to 33.3 kWh/kg H<sub>2</sub> and is known as the lower heating value (LHV) of water, with the difference between the two values equating to the latent heat of vaporisation of water [38]. With the products being in their elementary form, it is noted that the heat of formation of liquid water, 286 kJ.mol<sup>-1</sup>, equates to that of the heat of reaction or heat of combustion in relation to the water to hydrogen and oxygen reaction or vice versa [44]. As per Eq. 2-1, energy can be provided in two forms within an electrolyser to carry out the water electrolysis reaction, i.e. through heat and electrical input. The required electrical input (or usable work in a fuel cell) relates to the Gibbs free energy change of reaction which differentiates to the heat of reaction or enthalpy change of reaction by subtracting the multiple of the entropy change and the absolute temperature (Eq. 2-10) [39], [45].

$$\Delta G = \Delta H - T\Delta S \quad \text{Eq. 2-10}$$

The standard entropy change of the reaction depicted in, Eq. 2-1, equates to 0.163 kJ.mol<sup>-1</sup> [39], [44]. When multiplied by the absolute temperature the term equates to 48.68 kJ.mol<sup>-1</sup>. This equates the Gibbs free energy change to 237.2 kJ.mol<sup>-1</sup>. The Gibbs free energy and enthalpy change of reaction can therefore be reduced to an electrochemical potential, as per Eq. 2-11 and Eq. 2-12 [38], [39], [45], [46],

$$\Delta G = nFE_T \quad \text{Eq. 2-11}$$

$$\Delta H = nFE_{TN} \quad \text{Eq. 2-12}$$

where  $n$  is the number of electrons transferred in the reaction,  $F$  is Faraday's constant (96485 C.mol<sup>-1</sup>).  $E_T$  (also referred to as the reversible cell voltage  $E_{rev}$ ) relates to the thermodynamic potential required to split water at the specified operating conditions and  $E_{TN}$  is the thermoneutral voltages which stipulate the voltage at which sufficient energy has been provided to prevent heat absorption from the environment (endothermic). Consequently, operating between the thermodynamic and thermoneutral voltage would result in energy being absorbed from the environment to overcome the entropy energy deficit consequently resulting in a temperature drop of the electrolysis system. At standard temperature and pressure (STP) conditions  $E_T^o$  and  $E_{TN}^o$  equate to 1.23 V and 1.48 V [38], [46], [47]. The thermodynamic voltage, and consequently the Gibbs free energy change is dependent on temperature and the partial pressures of hydrogen, oxygen, and the activity of water. This relationship is described by the Nernst equation, Eq. 2-13 [38], [48].

$$E_T = E_T^o - \frac{RT}{nF} \ln \left( \frac{p_{H_2}^2 p_{O_2}}{\alpha_{H_2O}} \right) \quad \text{Eq. 2-13}$$

The enthalpy of reaction, and consequently the thermoneutral voltage, increases with temperature according to Kirchhoff's Law Eq. 2-14. A similar relationship is described for the change in entropy with changing temperature at set pressure (isobaric), Eq. 2-15 [44],

$$\Delta H = \int_{T_1}^{T_2} C_1(T) dT + L_v + \int_{T_2}^{T_3} C_2(T) dT \quad \text{Eq. 2-14}$$

$$\Delta S = \int_{T_1}^{T_2} \frac{C_1(T)}{T} dT + \frac{L_v}{T} + \int_{T_2}^{T_3} \frac{C_2(T)}{T} dT \quad \text{Eq. 2-15}$$

where  $C_1$  and  $C_2$  describes the liquid and gaseous heat capacities as a function of temperature of the species under investigation and  $L_v$  represents the latent heat of vaporisation. It is important to note that increasing the temperature at which the electrolysis reaction is performed would decrease the thermodynamic voltage (Gibbs free energy change of reaction), however, it would increase thermoneutral voltage. According to Eq. 2-10, for the thermodynamic voltage (Gibbs free energy of reaction) to decrease, the entropy and absolute temperature multiplication term would need to increase in magnitude with temperature at a greater rate than the enthalpy term.

**Table 2-1: Thermodynamic parameters at STP for the water electrolysis/hydrogen combustion reaction (Extracted from [44] – Permission Granted in Appendix G)**

| Compound     | $\Delta G_f^\circ (\frac{kJ}{mol})$ | $\Delta H_f^\circ (\frac{kJ}{mol})$ | $S^\circ (\frac{kJ}{mol.K})$ | $L_v (\frac{kJ}{mol})$ | $C_p (\frac{J}{mol.K})$         |
|--------------|-------------------------------------|-------------------------------------|------------------------------|------------------------|---------------------------------|
| $H_2$        | 0                                   | 0                                   | 0.131                        | -                      | $27.27 + 0.00326T + 50000/T^2$  |
| $O_2$        | 0                                   | 0                                   | 0.205                        | -                      | $29.96 + 0.00418T - 167000/T^2$ |
| $H_2O_{(g)}$ | -                                   | -                                   | -                            | -                      | $30.00 + 0.01071T + 33000/T^2$  |
| $H_2O_{(L)}$ | 237.2                               | 285.8                               | 0.07                         | 40.7                   | 75.44                           |

Figure 2-1 depicts the change in the enthalpy of reaction, Gibbs free energy and entropy, with temperature. From this figure, the power consumption gradient, as a function of temperature, can be assessed for each term in Eq. 2-10.

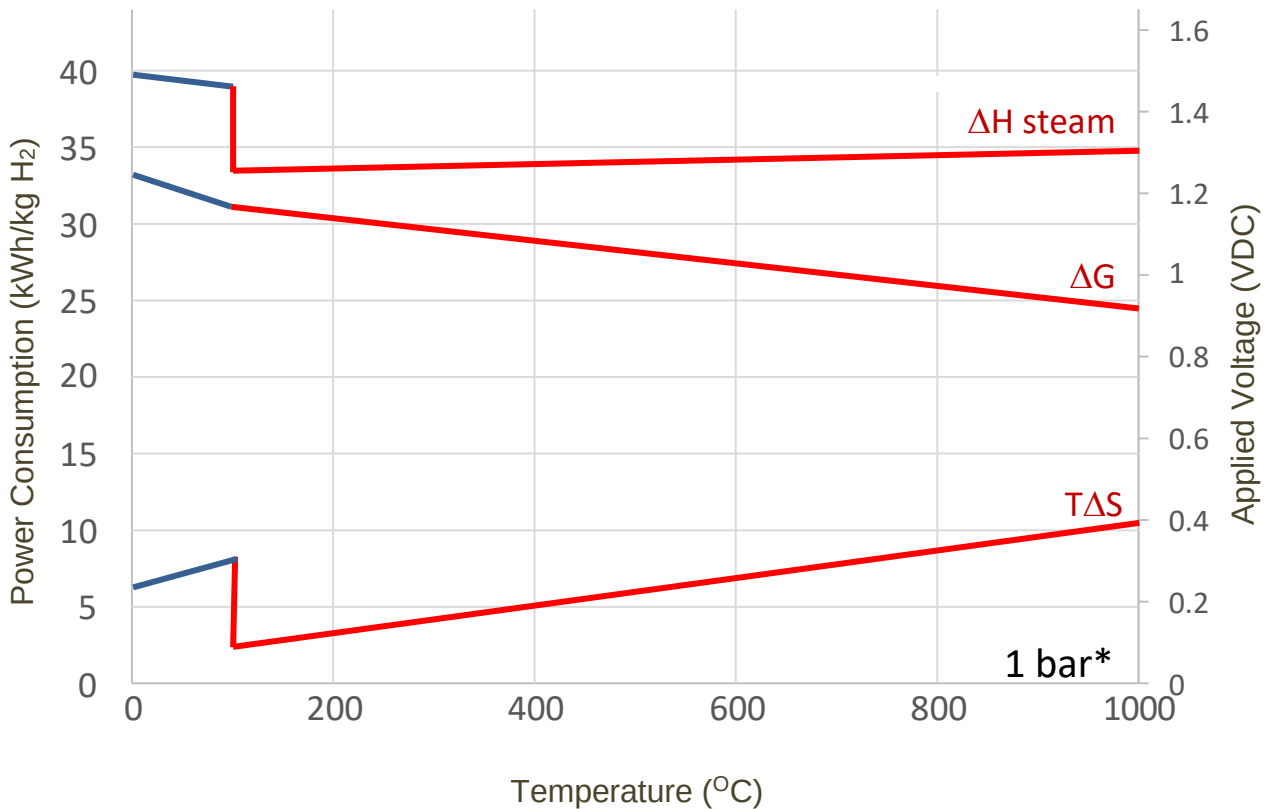


**Figure 2-1: The change in the thermodynamic parameters for the water electrolysis/hydrogen combustion reaction with temperature.**

From Figure 2-1, it is evident that the Entropy term does increase in magnitude with temperature at a rate that is greater than the increase of the enthalpy term. This result is expected as the entropy is a direct multiplication between the entropy change and the absolute temperature

wherein the increase in the enthalpy term is a consequence of the multiplication between the lower valued heat capacity of water and the absolute temperature. The reduction in the thermodynamic voltage (Gibbs free energy) indicates that less electrical input (electrical energy consumption) is required to split water at higher temperatures. A system operating at higher temperatures is capable of operating at lower voltages, hence, higher efficiencies, as less energy will be removed from the system as heat. This concept presents an area of potential for a membraneless electrolyser (such as DEFT™) as the temperature limited membrane/diaphragm has been removed from the system.

### 2.1.2 Cell Resistances and Overpotentials

The overall reaction has a standard reduction potential of 1.23 V at STP conditions. As stated, this equates to a minimum electrical energy requirement of 237 kJ to dissociate one mole of water molecules [39], [44]. In an electrolytic cell, greater potential differences, hence greater electrical energy requirements are needed to overcome the resistances for electron transfer. This additional energy requirement is known as the overpotential, which may be defined as the applied voltage above that of which is thermodynamically required to drive the reaction. Overpotential is required to overcome activation energy barriers, concentration gradients, junction potentials and other associated resistances. The overall voltage of an alkaline electrolysis cell can be represented as per Eq. 2-16 [33], [46],

$$R_{cell} = E_{Rev} + \eta_{anode}(j) + \eta_{cathode}(j) + IxR_{ohmic}(j) \quad \text{Eq. 2-16}$$

where  $E_{Rev}$  is the reversible cell potential (thermodynamic volage),  $\eta_{anode}$  and  $\eta_{cathode}$  the cathodic and anodic overpotential, and  $IxR_{ohmic}$  being the multiple between the current and the various sources of cell resistances (resistance to charge transfer). The anodic and cathodic overpotential is best described by the Butler-Volmer equation. The Butler-Volmer equation describes the dependence of the current density on the surface potential of an electrode and the adjacent electrolyte for a single-step redox process, Eq. 2-17 [41], [46],

$$j = \overrightarrow{j_a} + \overleftarrow{j_c} = nF\overleftarrow{k_o}C_R e^{\left(\frac{\alpha_a nF(E-E^0)}{RT}\right)} - nF\overrightarrow{k_o}C_O e^{\left(\frac{\alpha_c nF(E-E^0)}{RT}\right)} \quad \text{Eq. 2-17}$$

where  $\overleftarrow{k_o}$  and  $\overrightarrow{k_o}$  are the rate constants of the forward and reverse process of the single-step reaction,  $\alpha_a$  and  $\alpha_c$  are the exchange coefficients of the oxidation (anodic) and reduction (cathodic) processes and  $C_R$  and  $C_O$  refers to the concentration of species to be reduced and

oxidised.  $\alpha_a$  and  $\alpha_c$  are fractional values which are related such that their summation equates to 1. In general, both the oxidation and reduction exchange coefficients are equal and therefore equate to 0.5 [41], [46], [49]. Assuming the concentration at the interface of the electrode is equivalent to that of the bulk solution (i.e. no mass transfer limitations) and substituting for the definition of overpotential ( $\eta_{anode} = E - E^o$ ), Eq. 2-17 reduces to Eq. 2-18 [38], [41], [49],

$$j = j_0 \left( e^{\left( \frac{\alpha_a n F \eta}{RT} \right)} - e^{\left( \frac{\alpha_c n F \eta}{RT} \right)} \right) \quad \text{Eq. 2-18}$$

where  $j_0$  is the exchange current density. Further to this, at high negative and positive potentials (high overpotentials) the Butler-Volmer equation can be reduced to the Tafel equation as per Eq. 2-19, where  $\beta$  represents the Tafel slope [38], [41], [49], [50].

$$|\eta| = \beta \frac{\log(|j|)}{\log(j_0)} \quad \text{Eq. 2-19}$$

The exchange current density and the Tafel slope is dependent on the nature of the electrode. Consequently, the performance of the electrode depends on characteristics such as coating/catalyst material selection (affecting reaction pathways and activation energies), surface properties (affecting electrode area and bubble adhesion), structure and support material, etc.

The sum of the resistance to charge transfer represented as  $R_{ohmic}$  in Eq. 2-16, is shown by Eq. 2-20 [41], [46],

$$R_{ohmic} = R_{circuit} + R_{O_2,Bubble} + R_{anolyte} + R_{membrane} + R_{catholyte} + R_{H_2,Bubble} \quad \text{Eq. 2-20}$$

where the  $R_{circuit}$  is the electrical resistance associated with the external electrical circuit which is a function of conductor material (material resistivity) and conductor dimensions.  $R_{anolyte}$ ,  $R_{catholyte}$ , and  $R_{membrane}$  is the resistance to mass transfer experience within the liquid electrolyte and membrane/diaphragm separator,  $R_{O_2,Bubble}$  and  $R_{H_2,Bubble}$  being the resistance to ion transfer as a consequence of bubble formation thus creating voids within the electrolyte and thus reducing the area of the electrode-electrolyte interface. Depicted in Figure 2-2 is the contribution of each parameter (defined in Eq. 2-16) to the total overpotential applied to an alkaline unipolar cell to obtain set current densities utilising unactivated nickel electrodes [51].

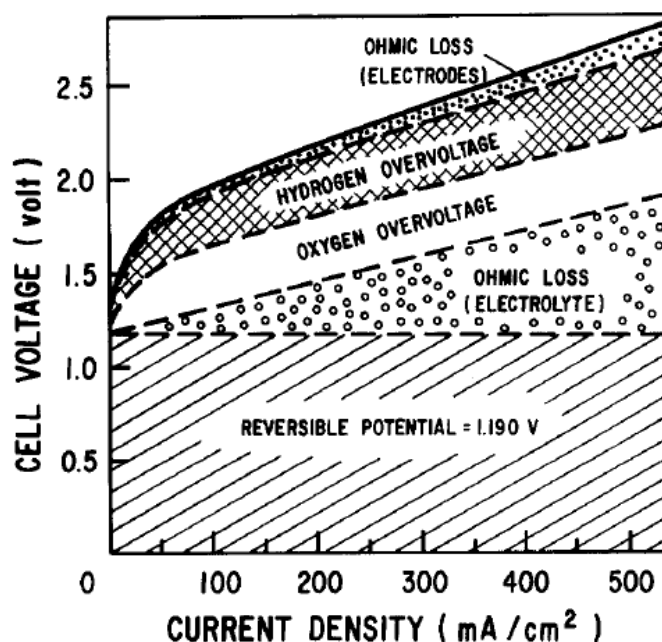


**Figure 2-2: Overpotential contributions in a unipolar alkaline cell operating with unactivated nickel electrode at temperatures above that defined by STP (Extracted from [51] – Permission Granted in Appendix G)**

From Figure 2-2, at low current densities, the hydrogen and oxygen account for the largest contribution of overpotential, however, the contribution of the electrolytic ohmic losses dominates at higher current densities. This is expected as with higher current densities bubble void fraction in the electrolyte, bubble coverage of electrode area, concentration gradients and further mass transfer limitations become apparent.

### 2.1.3 Electrolysis Efficiencies

The efficiency of an electrolysis system is a key parameter as it ultimately determines to what extent energy is “wasted” during the hydrogen and oxygen production process. It is of particular importance in areas where hydrogen is to be used as an energy storage medium as the ultimate goal is to capture and later release as much of the original energy captured as possible. In such a case both the efficiency of the generation system (electrolyser system) and the utilisation system (fuel cell) needs to be optimised.

In systems where both an electrical input and a heat source are supplied to the system, the determination of system efficiencies gathers some complexities, however, in the case of conventional PEM and alkaline systems where electrical energy is supplied to carry out the reaction the calculations are relatively simple as it is based mainly on the electrolyzers operating

voltage and the power consumption of the balance of plant components. There does, however, exist several efficiency terms that relate to the defined system boundary and/or the basis of efficiency determination. There have been efforts within the electrolysis industry to attempt to standardise efficiency determinations, however, some ambiguity still exists in system boundary selection. Figure 2-3 shows a schematic of an electrolysis plant of which various system boundaries can be defined.

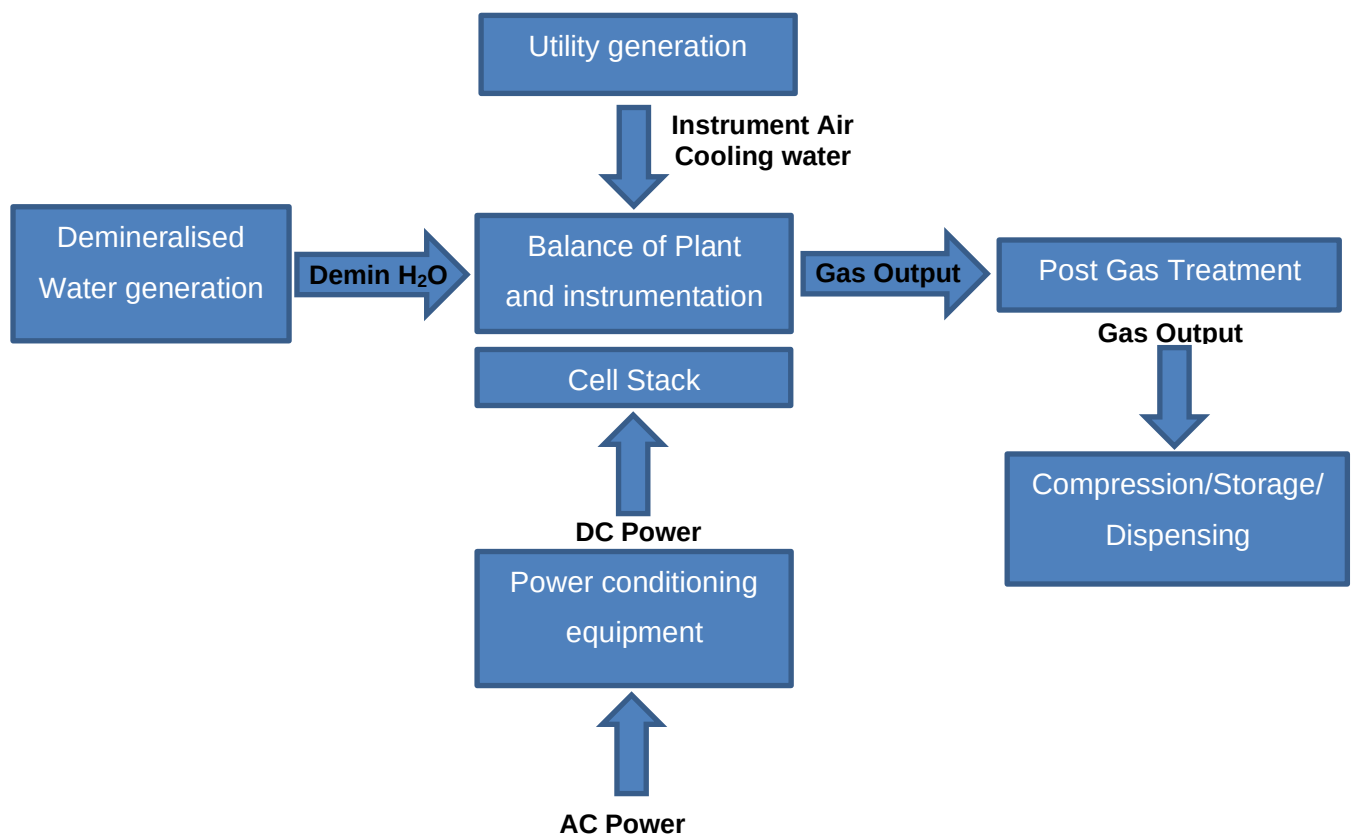


**Figure 2-3: Schematic showing sections of an electrolysis plant.**

Stack efficiencies involve a system boundary around the electrolysis stack and are based purely on the operating potential. A system boundary can be drawn around the stack and balance of plant taking into account the stack power consumption and that of auxiliary equipment and instrumentation. This can either include or exclude the efficiency of the rectifier system, hence, working off the determination of DC input or AC input efficiency. Lastly, an overall plant efficiency can be determined, however, for fair assessment/comparison further information relating to the stack and input and output parameters needs to be provided.

There are several ways to represent stack efficiencies. This includes both the voltage and thermal efficiency of the electrolyser stack, as per Eq. 2-21 and Eq. 2-22, and is based purely on operating

potentials [28], [33], [46]. The losses can be redefined as the additional overpotentials applied to the cell.

$$\varepsilon_{volatge} = \frac{\Delta G}{\Delta G + losses} = \frac{E_{Rev}}{E_{cell}} \quad At \ STP \ ... = \frac{1.23 \ (V)}{E_{cell}} \quad Eq. \ 2-21$$

$$\varepsilon_{volatge} = \frac{\Delta H}{\Delta G + losses} = \frac{E_{Rev}}{E_{cell}} \quad At \ STP \ ... = \frac{1.48 \ (V)}{E_{cell}} \quad Eq. \ 2-22$$

The hydrogen faradaic efficiency is another well-established efficiency term that is defined as the ratio of the actual mass or volume of hydrogen gas recovered at the edge of the defined system boundary over the maximum theoretical mass or volume of hydrogen gas produced. This efficiency term takes into account losses due to the existence of shunt and leakage currents and losses due to gas diffusion through the membrane/diaphragm and electrode gap structures. Depending on the extent of the system boundary this efficiency value may also include product gas losses through sampling systems, potential process connection leaks and or venting systems (as per Eq. 2-23) [6], [52].

$$\varepsilon_{Faraday} = \frac{V_{measured}}{V_{Max \ Theoretical}} = \frac{m_{measured}}{m_{Max \ Theoretical}} \quad Eq. \ 2-23$$

The maximum theoretical mass of hydrogen produced can be determined with Eq. 2-24, where  $I_{uni}$  is the unipolar current, which in a bipolar configuration can be determined by multiplying the cell current with the number of electrode pairs.  $M_{H_2}$  is the molar mass of hydrogen, and  $t$  is the time variable defined by the production rate period [28].

$$m_{H_2} = \frac{M_{H_2} I_{uni} \cdot t}{nF} \quad Eq. \ 2-24$$

The stack voltage, however, does not indicate power consumption of the balance of plant and other auxiliary units. This information is critical as high parasitic loads, such as those defined in flow systems, can render the overall hydrogen generation process inefficient even though the stack alone is showing a high-efficiency value. Two efficiency values are common in overall system efficiency determinations, i.e. the HHV and LHV efficiency. In both cases, the HHV or the LHV respectively, is ratioed to the overall power input defined by a system boundary (as per Eq. 2-25 and Eq. 2-26).

$$\varepsilon_{HHV} = \frac{HHV^o}{Overall \ power \ consumption} = \frac{39.4}{Overall \ power \ consumption} \quad Eq. \ 2-25$$

$$\varepsilon_{LHV} = \frac{LHV^o}{\text{Overall power consumption}} = \frac{33.3}{\text{Overall power consumption}} \quad \text{Eq. 2-26}$$

## 2.2 Water Electrolysis Systems

Three commercially available electrolysis technologies currently exist, namely, alkaline electrolyzers, ion-exchange electrolyzers (both proton and anion) and solid-oxide electrolyzers. A great deal of literature has been generated comparing these technologies with a greater interest being placed on PEM and Alkaline comparisons [4], [19], [20], [25]–[27], [53], [54], while alkaline and ion-exchange systems are currently the most viable and commonly implemented industrial solutions. Between PEM and liquid alkaline systems, the alkaline water electrolyser has seen the greatest market penetration with over 400 electrolyzers seen in operation in the year 1902 [55]. This is accredited to the fact that alkaline systems are the most robust and reliable of the available electrolysis technologies. Alkaline electrolyser systems offer high efficiencies >70% HHV at a reduced CAPEX and increased lifespan when compared to the proton exchange (PEM) systems due to their ability to use lower-cost non-noble materials of construction and electrocatalysts. PEM systems, however, offer higher current densities (higher production rates per volume of device) and are considered to be of quick response exhibiting short start-up cycles thus handling load fluctuations well. These characteristics have set out PEM systems to be better suited for linkage to renewables and more practical for use in cases that require on-demand flexible hydrogen production [42]. Anion-exchange membrane electrolyzers (AEM's) and zero-gap liquid alkaline system have, however, recently been introduced into the market [50], [55], [56]. Both work to reduce cell resistances through electrode gap reduction and reduction/removal of bubble resistances, thus, attempting to capitalise on the advantages associated with PEM cells. This allows for current density increases while still maintaining the ability to utilise more cost-effective and durable materials of construction. Although SOE systems can operate at high stack efficiencies by operating at temperatures of 700 – 900°C, there are no notable commercially utilised systems deployed in a commercial application. This is mainly due to high cost, limited durability, sealing issues and the fact that SOE systems may be limited to operation from renewable heat or wasted heat sources [4]. Consequently, the technology is still very much in the laboratory development phase.

What is common amongst all three technologies is that they all employ some kind membrane/diaphragm. The main function of which is to separate the produced hydrogen and oxygen gas while still permitting the mass transfer of ions between the cathodic and anodic compartments. Although the technologies operate within different environments all three incorporate a unique version of the membrane/diaphragm that is designed to permit the transport

of specific ions that are unique to their operating environment (i.e. their specific half-reactions). The function of the separator is, therefore, unique to each technology operating principle.

### 2.2.1 Liquid Alkaline Operating Principle.

In a conventional alkaline system, a liquid KOH or NaOH electrolyte is utilised as a charge carrier. The system, therefore, operates within a corrosive alkaline environment. To keep the produced gases separated, porous diaphragms are incorporated in the setup. These porous diaphragms are hydrophilic and work on the principle of retaining liquid electrolyte within microchannels. The liquid electrolyte within the porous diaphragm structure gives the diaphragm its ionic conductivity [31]. The size of the microchannels pore size is in the micron scale hence providing a high bubble pressure and low gas permeability [57]. The fact the material itself is not responsible for ion conductivity, but the electrolyte contained within, results in an increase in area-specific resistance compared to that of the pure liquid electrolyte in accordance with the diaphragms porosity [33].

Up until the late 1900s asbestos was used as diaphragm material, however, due to its instability at high temperatures and its recent restrictions, due to associated health concerns, the industry has been encouraged to develop better-suited alternatives [31], [57]. Modern-day diaphragms incorporate Polyphenylene sulphide (PPS) materials, such as PPS felt, and composite materials. The AWE diaphragm that is most readily utilised is that of Zirfon® Perl manufactured by AGFA. This material is a ceramic composite structure consisting of 85% Zirconium dioxide ( $ZrO_2$ ) and 15% polysulphone material supported on a PPS mesh [31], [58].

**Table 2-2: Properties of Zirfon® Perl UTP 500, manufactured by AGFA  
(Extracted from [31] – Open Access)**

| Properties                                        | Values      |
|---------------------------------------------------|-------------|
| Thickness (um)                                    | 500 ± 50    |
| Maximum operating continuous temperature (°C)     | 110         |
| Porosity                                          | 50 ±        |
| Bubble point (bar)                                | 2 ± 1       |
| Gas permeability (l/min.cm <sup>2</sup> at 5 bar) | 4 ± 1       |
| Pore Size                                         | 0.15 ± 0.05 |
| Ionic Resistance (ohm.cm <sup>2</sup> )           | <0.3        |
| Maximum current density (kA/m <sup>2</sup> )      | 20          |

Operating temperatures in AWE systems normally extend to 80°C, however, the normal range is 60 – 90°C. This operating point allows for current densities of 0.2 – 0.4 A.cm<sup>-2</sup> at a voltage range of 1.8 to 2.4 VDC [19], [25] resulting in HHV stack efficiencies of 82% - 62% (47.9 – 63.8 kWh/kg H<sub>2</sub>). The extreme alkaline environment requires the use of nickel and stainless steel as electrode materials and for the balance of plant component manufacture [59]. Advanced alkaline systems that incorporate advanced catalyst coatings tend to avoid stainless steels due to the sensitivity of the catalyst to the existence of leachables such as iron (Fe) that may leach from stainless steel components. The iron contaminates the catalyst by reducing on the cathode or contaminates other system components through particulate build-up.

Maintaining a potential difference across the cell encourages the reduction of water on the cathode to form hydrogen gas and hydroxide ions. For an electrical circuit to be completed within the cell, and for the anodic and cathodic electrode compartment to maintain the same degree of charge, mass transfer of the hydroxide ion from the cathodic to the anodic compartment is required. Hydroxide ions, therefore, need to travel through the cathodic electrode gap, the porous diaphragm membrane, and the anodic electrode gap to later oxidise at the anode. Not only does bubble formation within the liquid electrolyte provide resistance to this mass transfer but the free movement of ionic agents in the liquid leads to the formation of what is known as a double-layer. The double-layer consists of ions of different charges aligning themselves in an ordered array along the surface of the electrode. This process is a non-faradaic process of capacitance build-up within the cell. A slight drop in potential is noted across this layer thus exposing the bulk solution to lower operating potentials and hence further electrical losses. The above-mentioned phenomena all culminate into lower operating current densities compared to their PEM counterparts [46].

To maintain effective temperature control and concentration setpoints within the cell, the liquid electrolyte is recirculated with subsequent removal of the produced hydrogen and oxygen gas in separate gas-lye separation vessels. The anolyte and catholyte is either recombined post gas separation or kept separate with an interlink between the hydrogen and oxygen separator vessels to assist in maintaining the level and concentration setpoints. A basic schematic of a liquid alkaline cell electrode assembly is provided in Figure 2-4.

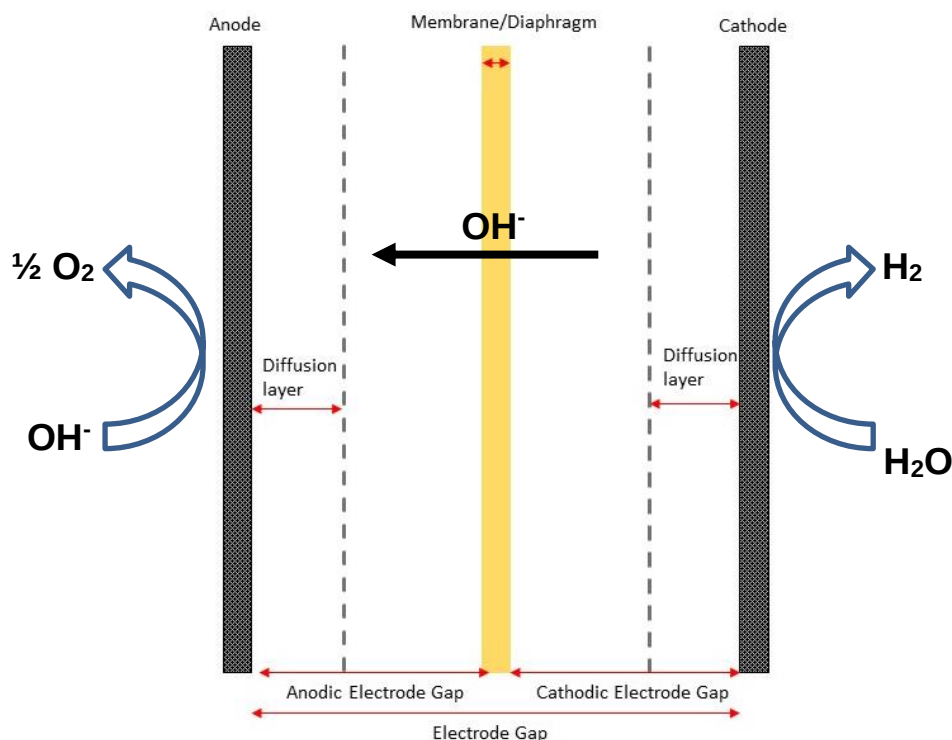


**Figure 2-4: Schematic showing the basic cell structure of an alkaline electrolyser**

In conjunction with the issue of low current densities (high cell resistances) experienced in liquid alkaline cells, these systems experience pressure and load range limitations. At low partial loads, unwanted gas diffusion remains prevalent, however, less product gas is generated resulting in a substantial increase in  $\text{H}_2$  in the  $\text{O}_2$  stream and vice versa. This is of particular concern when unwanted gas contaminants approach that of the lower or higher explosive limit.

### 2.2.2 Proton Exchange Membrane Operating Principle.

The proton exchange membrane electrolyser, first developed in 1966 by General Electric [60], was developed to address many of the issues associated with liquid alkaline systems. PEM systems do not make use of liquid electrolyte, but rather incorporates an acidic ion-exchange membrane. The capability of the ion-exchange membrane to transport ionic agents from the anodic to the cathodic compartment is not reliant on the porosity of the structure, and the liquid electrolyte contained within, but rather on its ability to transfer protons across a chain of perfluoro-sulfonic acid (PFSA) type functional groups incorporated into the structure of the membrane [4], [61] Consequently, the system does not require the use of a liquid electrolyte and therefore only a feed of demineralised water is required. Nafion<sup>®</sup>, developed by Du Point, is the most widely utilised acidic ion-exchange membrane in industry, however, other well-known brands, such as

Flemion®, Fumapem® and Aciplex® are available [20], [27], [62]. These ion-exchange membranes are thinner than their porous diaphragm alkaline counterparts with average thicknesses of 100 – 200  $\mu\text{m}$  with ion (proton) conductivities in the range of 0.1 – 0.2  $\text{S}\cdot\text{cm}^{-1}$  [63]–[66].

Due to the low porosity of the ion-exchange membrane, high gas purities of > 99.99%  $\text{H}_2$  are achieved and therefore not only reducing the need for downstream purification, but also improving process safety [55]. This reduction of gas diffusion across the membrane further allows for higher operating pressures around 30 to 50 barg [60], [62], [67], however, pressures of up to 150 – 200 barg have been achieved [55], [68].

The low gas permeabilities and dynamic operation associated with PEM systems allow for the ability to run off intermittent loads as gas purities are not seen to drop off at lower current densities. Further to the safety and gas quality improvements over tradition liquid alkaline cells, the electrodes in PEM electrolyzers are pressed against the membrane, hence, a “zero-gap” configuration results. This eliminates the phenomena of gas bubbles forming in the region between the cathode and anode thus preventing escalation in cell resistances through increases in the void fraction [69]. Current collectors (also known as gas diffusion electrodes) are utilised to supply power to the electrodes, provide support to the MEA and to control gas and liquid diffusion within the cell [27], [59]. A schematic representation of the cell is provided in Figure 2-5.

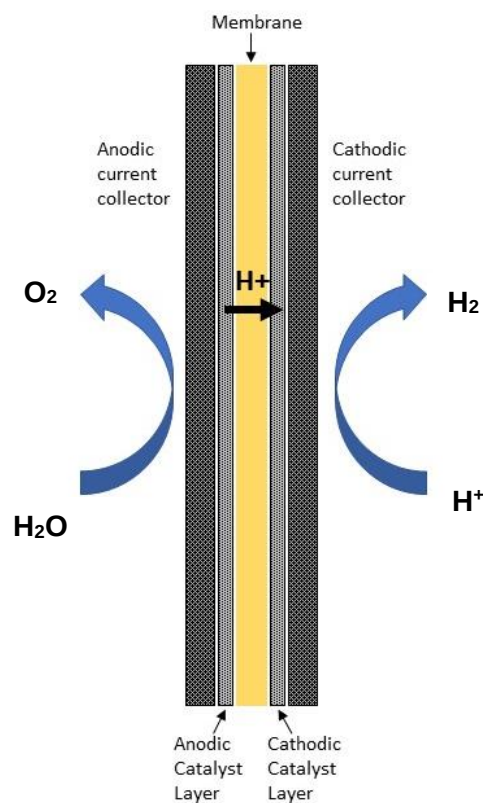


**Figure 2-5: Schematic showing the basic cell structure of a PEM electrolyser**

The high acidic environment associated with the use of perfluorosulphonated membranes requires the use of noble (platinum group) metals, in particular, platinum on the cathode and platinum or iridium on the anode [67], [70]. Typical platinum mass loadings fall within 0.8 – 1.0 mg Pt/cm<sup>2</sup> and iridium mass loadings of 2.0 – 2.4 mg Ir/cm<sup>2</sup> [60], [67]. Together with the reduced membrane thickness, incorporation of noble electrocatalysts and reduced cell resistances, PEM electrolyzers are capable of achieving higher current densities compared to liquid alkaline cells. At voltages of 1.8 – 2.2 VDC current densities of 0.6 – 2.0 A/cm<sup>2</sup> are noted as mean performance points [20], [59].

Although PEM electrolyzers carry many advantages over alkaline cells, they do have several associated drawbacks. The required use of PGM's results in high stack cost thus requiring a substantial capital investment for the purchase of these units. Secondly, the ion-exchange membranes utilised in PEM systems have a reduced lifespan, when compared to alkaline systems, consequently requiring replacement/stack overhaul within 10 000 – 50 000 operating hours [4], [20], [67]. The impact of the high capital cost and frequent cell maintenance schedules results in the need for stacks to operate at increased voltages to offset the high capital cost as this works to reduce stack sizes. In summary, the high capital cost works to drive the optimal CAPEX vs OPEX (overall cost of hydrogen) point to higher operating potentials. Consequently, with PEM systems operating at similar potentials to alkaline stacks, while carrying higher CAPEX requirements, results in similar, or in some cases, higher costs to produce hydrogen. Much effort has been extended to the development of an alkaline anion-exchange membrane electrolyser, however, this technology is still in the laboratory/early small commercialisation stage as intrinsic issues, such as poor membrane durability, low current densities and high catalyst loadings, still need to be solved for the technology to attain extensive market penetration [56].

### **2.2.3 Techno-Economic Comparison and Key Performance Parameters**

Although all the water electrolysis technologies are all subjected to the same thermodynamic limitations, the different operating environments and consequently the variable use of compatible materials allows the various approaches to achieve different performance values. This results in the different technologies having different CAPEX vs OPEX considerations and different niche areas of favourable operations. Each technology, therefore, has different techno-economic considerations, which ultimately affects the overall costs to produce electrolytic hydrogen in various applications. It is therefore worth noting that both alkaline and acidic technologies have respective advantages and disadvantages, however, these do not qualify or disqualify either

system as the more effective hydrogen production technology, but rather categorises each technology to specific end-use applications based on required operating conditions.

It is also important to assess the performance of current technologies to identify possible areas for improvement. Table 2-3 summarises the performance parameters for alkaline, PEM and AEM technologies. These are averaged values recorded for systems ranging from small scale to large scale production. Values for AEM systems are primarily sourced from lab-scale experiments, as very few systems have been released into the market that can be used for research.

**Table 2-3: Techno-economic specifications of various use cases of small scale alkaline and PEM systems**

| PARAMETER                                          | AWE                                                    | REF                  | PEM                             | REF                  | AEM                                   | REF                  |
|----------------------------------------------------|--------------------------------------------------------|----------------------|---------------------------------|----------------------|---------------------------------------|----------------------|
| <b>Electrolyte and Ionic Agents</b>                |                                                        |                      |                                 |                      |                                       |                      |
| <b>Electrolyte</b>                                 | 20-30% KOH                                             | [19]<br>[20]         | Perfluorosulfonated acid (PFSA) | [19]<br>[20]         | Quaternary Ammonia Polysulfone (QAPS) | [56]<br>[71]         |
| <b>Charge carrier</b>                              | OH <sup>-</sup>                                        | [19]<br>[20]         | H <sup>+</sup>                  | [19]<br>[20]         | OH <sup>-</sup>                       | [56]                 |
| <b>Recirculating liquid component</b>              | Potassium Hydroxide                                    | [26]                 | Deionised Water                 | [26]                 | Deionised water                       | [56]                 |
| <b>Separator</b>                                   | ZrO <sub>2</sub> with Polysulfone binder – Zirfon Perl | [20]                 | PFSA – e.g. Nafion              | [20]                 | QAPS                                  | [56]                 |
| <b>Materials</b>                                   |                                                        |                      |                                 |                      |                                       |                      |
| <b>OER catalyst</b>                                | Ni, Co, Based                                          | [20]<br>[25]         | Ir/Ru Oxide, Platinum           | [20]<br>[25]         | Ni, Pt, Cu Based                      | [56]                 |
| <b>HER catalyst</b>                                | Ni, Mo Based                                           | [20]<br>[25]         | Platinum                        | [20]<br>[25]         | Ir, Ni, Pd based                      | [56]                 |
| <b>Current collector and containment materials</b> | Nickel                                                 | [20]                 | Titanium, Stainless steel       | [20]                 | Nickel                                | [56]                 |
| <b>Operating Conditions</b>                        |                                                        |                      |                                 |                      |                                       |                      |
| <b>Nominal operating voltage (VDC)</b>             | 1.8 – 2.4                                              | [17]<br>[38]         | 1.8 – 2.2                       | [17]<br>[38]         | 1.8 – 2.2                             | [56]                 |
| <b>Current density (A/cm<sup>2</sup>)</b>          | 0,1-1                                                  | [25]<br>[38]         | 1-2.5                           | [25]<br>[38]         | 0.2 – 1                               | [56]<br>[72]         |
| <b>Operating temperature (°C)</b>                  | 40 - 90                                                | [19]                 | 20 - 100                        | [19]                 | 50 - 70                               | [56]<br>[71]         |
| <b>Operating pressure (Bar)</b>                    | 0 - 30                                                 | [19]<br>[53]         | 0 - 350                         | [19]<br>[53]         | 0 - 30                                | [56]                 |
| <b>Hydrogen purity (vol%)</b>                      | 99.8 – 99.99                                           | [26]<br>[56]<br>[72] | 99.9999                         | [26]<br>[56]<br>[72] | 99,99                                 | [26]<br>[56]<br>[72] |

|                                                         |                 |                      |                        |                      |                               |              |
|---------------------------------------------------------|-----------------|----------------------|------------------------|----------------------|-------------------------------|--------------|
| <b>Maximum load<br/>(%full load)</b>                    | 100             | [53]<br>[59]         | 160                    | [53]<br>[59]         | -                             | -            |
| <b>Minimum part load<br/>operation<br/>(%full load)</b> | 20              | [53]                 | 0                      | [53]                 | -                             | -            |
| <b>Warm start time</b>                                  | 5 min           | [53]                 | 10 s                   | [53]                 | -                             | -            |
| <b>Cold start time<br/>(min)</b>                        | < 60 min        | [25]                 | <20                    | [25]                 | -                             | -            |
| <b>Response time</b>                                    | Sec             | [72]                 | Milsec                 | [72]                 | -                             | -            |
| <b>Efficiencies and Power Consumption</b>               |                 |                      |                        |                      |                               |              |
| <b>Electrical input<br/>(kWh/kg H<sub>2</sub>)</b>      | 48 - 68         | [53]                 | 54 - 68                | [53]                 | ± 58                          | [56]<br>[73] |
| <b>LHV%</b>                                             | 49 - 70         | [53]                 | 49 - 62                | [53]                 | ± 58                          | [56]<br>[73] |
| <b>Size, Lifespans and CAPEX</b>                        |                 |                      |                        |                      |                               |              |
| <b>Production rate<br/>(Nm<sup>3</sup>/hr)</b>          | 5 - 500         | [53]<br>[54]         | 1 - 650                | [53]<br>[54]         | Lab Scale/Small<br>commercial | [56]         |
| <b>System size<br/>(MW)</b>                             | <0.1 – 2.2      | [53]                 | <0.1 - 3               | [53]                 | Lab Scale/Small<br>commercial | [56]         |
| <b>Stack lifetime<br/>(h)</b>                           | 80 000 – 96 000 | [25]<br>[38]<br>[54] | 25 000 – 80 000        | [25]<br>[38]<br>[54] | -                             | -            |
| <b>System lifetime<br/>(years)</b>                      | 20 - 30         | [59]                 | 10 - 20                | [59]                 | -                             | -            |
| <b>Efficiency degradation<br/>(% per annum)</b>         | 0.25 - 1.5      | [53]                 | 0.5 – 2.5              | [53]                 | -                             | -            |
| <b>System cost<br/>(€/kW)</b>                           | 370 - 2400      | [19]<br>[20]<br>[53] | 700 - 3500             | [19]<br>[20]<br>[53] | -                             | -            |
| <b>Maintenance cost<br/>(%System Cost)</b>              | 2 - 3           | [53]                 | 3 - 5                  | [53]                 | -                             | -            |
| <b>Maturity</b>                                         | Mature          | [25]                 | Recently<br>Commercial | [25]                 | Demonstration/<br>R&D         | [56]<br>[72] |

The stack and system sizes stated in Table 2-3 are provided as an electrical load at a nominal capacity of the respective plants. PEM electrolyzers have recently produced the largest single stack, of approximately 3 MW, surpassing the single-stack production capabilities of alkaline technology [74]. Larger PEM and alkaline systems are achieved through the modularisation of stack units. Efficiencies are based on the Lower Heating Value (LHV) of hydrogen and include auxiliary equipment efficiencies. System boundaries for energy consumption and efficiency values include losses for AC-DC conversion. Additional purification and compression costs of hydrogen production are not included in the total energy consumption of the system. The electrical

efficiency of a stack is dependent on the current densities achieved by electrolyser stacks. High current densities at relatively low cell potentials will result in electrically efficient stacks, however, the system could be operated at higher potentials (lower voltage efficiencies) to reduce system CAPEX costs. The values quoted for system costs are, therefore, dependant on the stated voltage efficiency. Consequently, to provide a fair representation of a systems capital requirements a system efficiency or stack efficiency needs to be provided alongside system cost. The system cost values quoted in Table 2-3 are not stipulated alongside an efficiency point representing distinct system characteristics, but rather provides a summary of systems costs across an efficiency range and a small forecourt to the large forecourt size range. As a summary Table 2-4 offers a list of advantages and disadvantages associated with each technology.

**Table 2-4: Advantages and disadvantages of Alkaline, PEM and AEM technology ([27], [56], [59])**

| AWE                                 | PEM                                                 | AEM                           |
|-------------------------------------|-----------------------------------------------------|-------------------------------|
| Advantages                          |                                                     |                               |
| Mature technology                   | Higher current densities                            | Non-noble metal catalyst      |
| Non-PGM catalyst                    | Low operating voltages<br>(Good voltage efficiency) | Non-corrosive electrolyte     |
| Long Term Stability                 | Good partial load (full load range)                 | Compact cell design           |
| Low CAPEX                           | Rapid system response                               | Relatively low CAPEX          |
| Megawatt range                      | Compact cell design                                 | Sealed-off system – no leaks  |
| Cost-effective                      | Dynamic operation                                   | High operating pressure       |
| Robust operation                    | Megawatt range                                      |                               |
| Disadvantages                       |                                                     |                               |
| Low current densities               | High CAPEX                                          | Laboratory stage              |
| Crossover of gas (low gas purities) | Acidic corrosive components                         | Low current densities         |
| Poor dynamic operation              | Possible low durability                             | Rapid degradation of membrane |
| Corrosive liquid electrolyte        | Noble metal catalyst                                | High catalyst loading         |
| Low-pressure operation              | Strict water purification standards                 |                               |

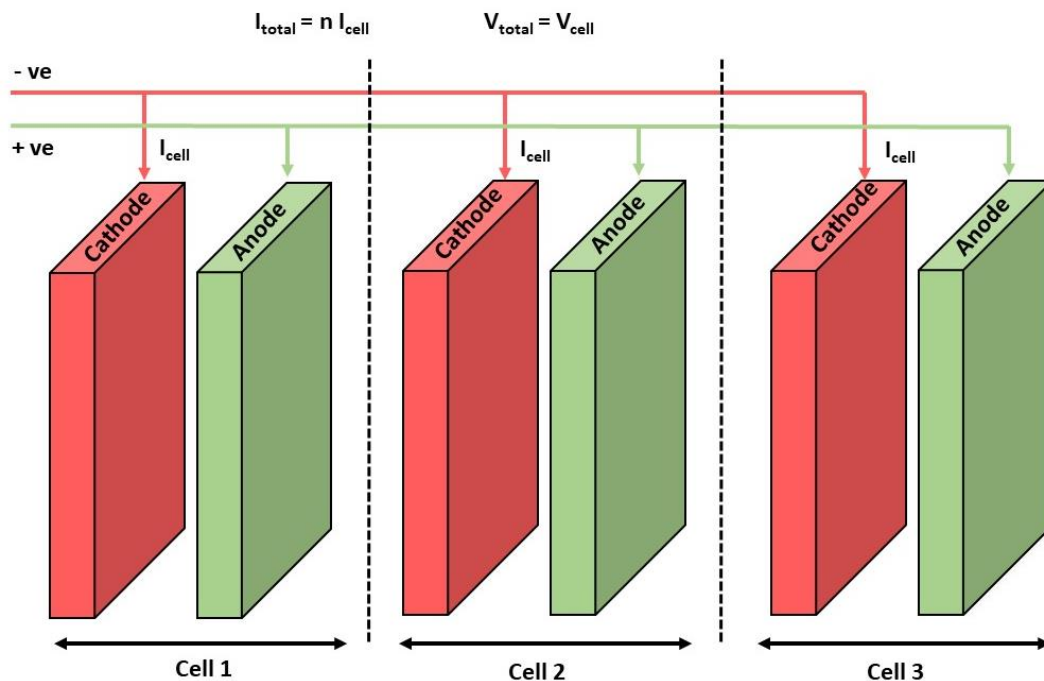
## 2.3 Liquid Alkaline Electrolyser Cell Configurations

Liquid alkaline cells are simple devices requiring only a few components in its construction. This includes conductive end/sealing plates, anodic and cathodic electrodes, a diaphragm/membrane separator material, liquid/gas seals, a liquid alkaline solution, and a means of current distribution/collection (bipolar plates or unipolar connections). How power is fed to the cell, conditions of the electrolyte and the configuration of the electrodes, are some of the major considerations when it comes to the design of liquid alkaline cells.

### 2.3.1 Bipolar or Unipolar

Liquid alkaline electrolyser stacks can be installed and electrically connected in two main configurations, parallel (unipolar connection) or series connection (bipolar connection), with a schematic showing the two connection variations in Figure 2-6.

a)



b)

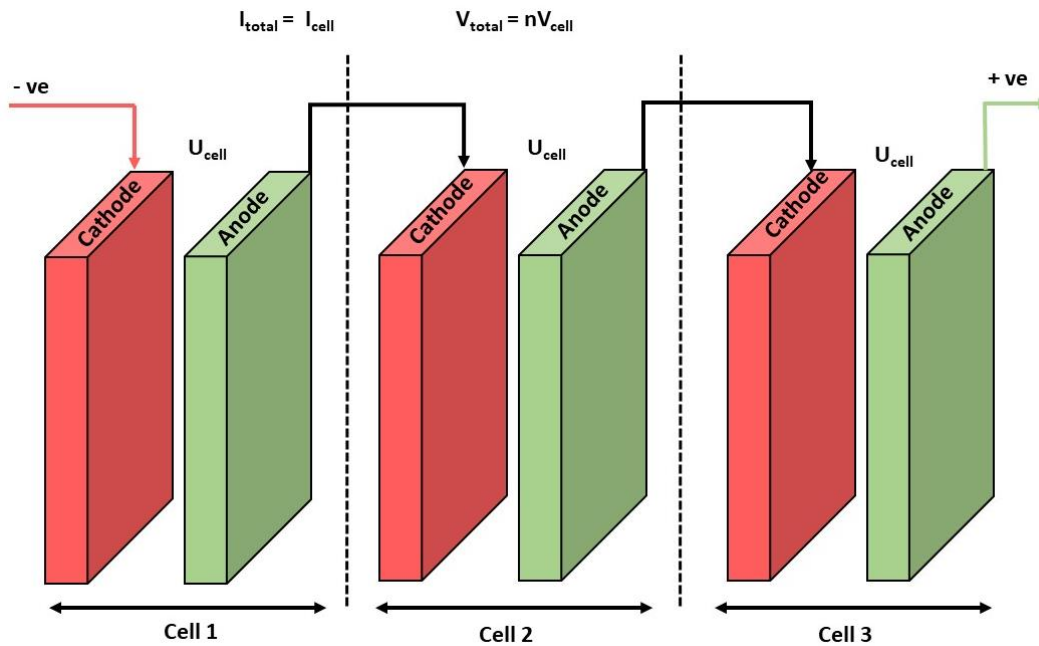


**Figure 2-6: Configuration for a liquid alkaline system electrolyser in a) Parallel (Unipolar) and b) Series (Bipolar) (adapted from [4])**

In the parallel/unipolar connection an electrical connection, from the power supply's positive and negative terminal, is made to each anode and cathode, respectively. In this configuration, the voltage/potential difference across each cell is maintained at the output voltage of the rectifier system and the current output from the rectifier is split amongst the number of cells in the stacks array. This results in a low voltage/high amperage operation. In the bipolar configuration, an anode and cathode make electrical contact, either through a current lead or pre-electrode, with a conductive plate. Electrical connections are made to either end of the stack (on the endplates). The high potential difference across the stack encourages polarisation of the bipolar plates whereby either surface of the plate takes on an alternating positive and negative potential. In this series connection, the voltage is split amongst the number of pairs in the stacks array and the series current is defined as the output current from the rectifier system. This configuration is therefore called bipolar as each plate takes on two polarities (a negative and positive charge on either side of the plate). This results in a high voltage-lower current operation [4].

Unipolar electrolyzers are also known as a tank electrolyzers, as the electrolyser is essentially a series of anodic and cathodic baths with individual gas collections [28]. They provide a simple and robust electrolysis method as each cell is self-contained/modular, therefore, a single cell can be taken offline for maintenance and repair. This results in a unipolar electrolyser being relatively low cost, but rather large and bulky. Each cell is self-contained therefore no leak/parasitic currents are noted in its operation resulting in high faradaic efficiencies.

Bipolar electrolyzers are configured in a filter press arrangement with an external pump being a requirement to provide flow to the stack. This tight setup allows for small electrode gaps and hence a low voltage operation due to lower cell resistances. Secondly, the filter press design extends itself to a higher temperature and pressurised operation. The low amperage and high voltage operation allow for low-cost busbar connections and power conditioning equipment. One of the main drawbacks of bipolar electrolysis stacks is that they allow for intercell current pathways therefore stray/parasitic currents can result [28]. With the voltages being summed across the cell, its length is limited by the overall cell voltage and the effect it has on driving parasitic currents within the cell. With the cost and space savings of the stack and power conditioning system associated with bipolar configurations, a greater uptake of this cell configuration is observed [28].

### 2.3.2 Electrolyte Considerations

In liquid alkaline cells the selection of the electrolyte and its conditions of operation, such as temperature and concentration, can have a presiding effect on the performance of the cell. The objective is to select an electrolyte that will not only act as an intermediate in the water dissociation reaction, therefore preventing side reactions and targeting only oxygen and hydrogen gas formation, but also exhibits a high conductivity. The resistivity of the electrolyte, and in turn the electrolyte's conductivity, is one of the largest contributing factors to the cell's resistance and ultimately the cell's performance (current density at specified voltage). For this reason, an electrolyte of choice must be optimised in terms of conditions and temperature such that its conductivity is maximised at these conditions.

Potassium hydroxide (KOH) and sodium hydroxide (NaOH) are commonly utilised in liquid alkaline cells. KOH is more frequently utilised as it exhibits a higher conductivity compared to that of NaOH [75]. Atmospheric liquid alkaline systems operate in the 70 – 90°C range, however, more frequently at 80°C [19]. It would therefore be beneficial to the performance of the electrolyser if the KOH concentration is selected such that the conductivity is maximised at this temperature. Gilliam, *et al.* in their paper “A review of specific conductivities of potassium hydroxide solutions for various concentrations and temperatures”, proposed a relationship between the conductivity of KOH and the temperature (T) and concentration of the solution (M), as per Eq. 2-27 [32]. This equation showed close correlation to experimental data in the 30 – 100°C range.

$$\kappa = -2.041(M) - 2.8 \times 10^{-3}(M^2) + 5.33 \times 10^{-3}(MT) + 207.2\left(\frac{M}{T}\right) + 1.04 \times 10^{-3}(M^3) + 3 \times 10^{-7}(M^2T^2) \quad \text{Eq. 2-27}$$

Data generated from Eq. 2-27 is provided in Figure 2-7 showing the dependence of KOH conductivity on temperature and concentration.

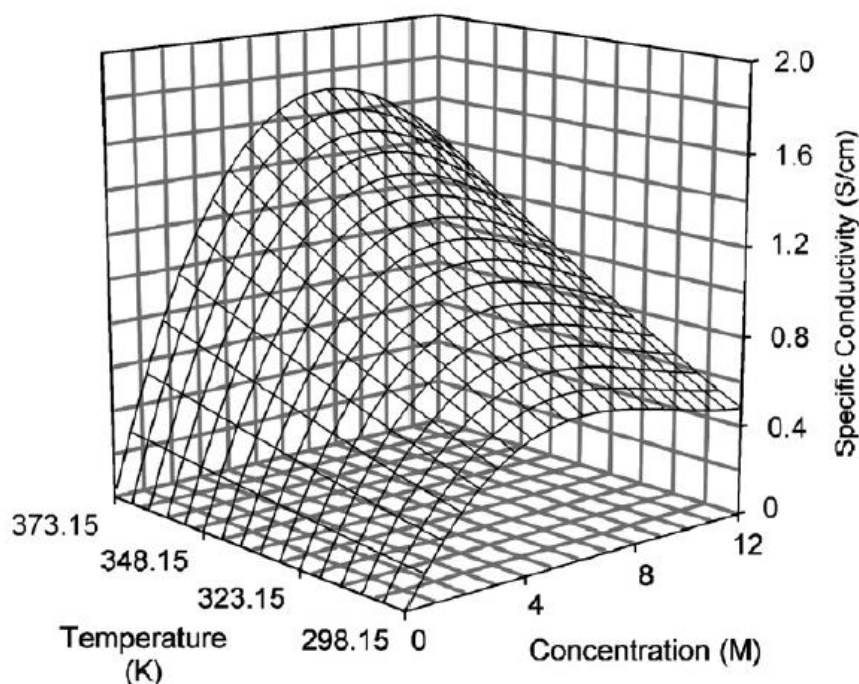


**Figure 2-7: KOH concentration with changes in temperature (K) and concentration (M)**  
**(Extracted from [32] – Permission Granted in Appendix G)**

Figure 2-7 notes that the conductivity of the potassium hydroxide increases with temperature and forms a parabolic curve with concentration. With increasing concentration more ionic species are present to act as charge carriers thus increasing the conductivity of the solution, however, this relationship exists up until a point at which a high concentration of ions starts to present limitations/resistance to mass transfer. Increasing the concentration above this point results in a decrease in solution conductivity. It is noted that at 80°C (353.15 K), the specific conductivity of potassium hydroxide is maximised at roughly 7 - 8 M, with a more narrowed-in weight percentage of 30 – 34 % [32]. This is in agreement with concentration setpoints noted in industrial installations of alkaline systems [19] [20].

### 2.3.3 Electrode Gap

As noted in Section 1.3.1, concentrated KOH electrolytes exhibit a higher conductivity, lower resistivity, when compared to ion-exchange membranes and diaphragms [76]. The actual cell resistance determination, however, is dependent on the distance the ions must travel between

the anode and cathode, i.e., the length of the electrode gap. An equation defining the resistivity to resistance relation is provided in Eq. 2-28. where  $\rho$  is the resistivity of the electrolyte,  $l$  is the thickness and  $A$  represents cross-section area.

$$R = \frac{\rho l}{A} \quad \text{Eq. 2-28}$$

Eq. 2-28, therefore, notes that even if the components within the electrode gap exhibit a lower resistivity, the overall cell resistance can be concluded to be higher provided that the electrode gap is sufficiently large. With commercial diaphragms reporting thicknesses in the range of 500  $\mu\text{m}$  [31] and commercial ion-exchange membranes reported between 100 – 200  $\mu\text{m}$  [76], membraneless systems would need to focus on electrode gap reduction to minimise cell resistances beyond that of commercial membrane/diaphragm systems. Gillespie, *et al.* presented data surrounding the effect of the electrode gap on cell performance in a membraneless electrolyser [1] and Phillips, *et al.* presented data for a similar study in a conventional liquid alkaline diaphragm cell utilising ULP500 Zirfon Perl® [33]. The results of both studies are provided in Figure 2-8.

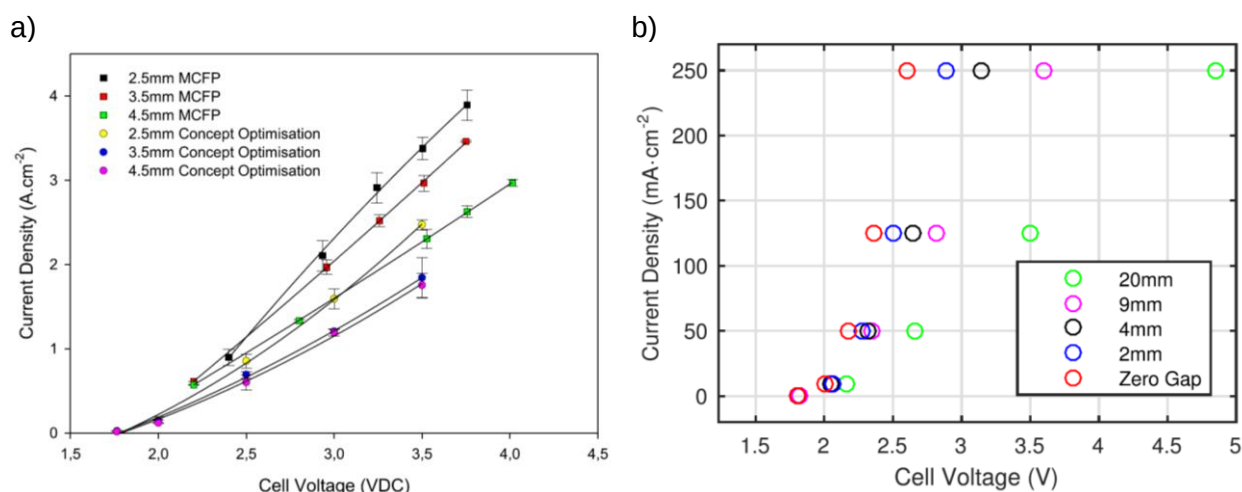


**Figure 2-8: IV data for variable electrode gap dimensions in a) a membraneless (Extracted from [1] – Permission Granted in Appendix G) and b) diaphragm (Extracted from [33] – Permission Granted in Appendix G) liquid alkaline cell.**

Both studies noted that the electrode gap had a substantial effect on cell performance with a membraneless cell noting a 30% increase in current density moving from a 3.5 mm to 2.5 mm gap [1]. A 12% reduction in cell voltage is noted at 250  $\text{mA}\cdot\text{cm}^{-1}$  moving from a 2.5 mm to zero gap design configuration in a conventional alkaline cell, represented in Figure 2-8b. Assessing

the performance increase in terms of current density, Figure 2-8b notes an almost 50% increase in current density moving from a 2 mm to zero gap configuration. The study in its entirety noted a mean 30% reduction in cell resistances moving from a 2 mm to zero-gap cell configuration [33].

With the associated benefits of minimising the electrode gap to a zero-gap configuration (i.e. reduced cell resistances, better bubble management and membrane/diaphragm support), this technology has received much attention over the past decade [20], [33], [40], [50]. The setup intends to press the electrodes against the diaphragm separating structure to prevent a “bubble curtain” from forming within the electrode gap that works to reduce cell resistance at low and, in particular, high current densities. The extent, or the force, at which the electrodes are pressed against the membrane needs to be optimised such that electrode area is not significantly blocked by the diaphragm, but still ensuring that the electrode makes sufficient contact with the separator. This parameter is difficult to control and often requires that the stacks be constructed such that sealing is not a function of endplate compression.

## **2.4 Membraneless Water Electrolysis Systems**

There has been much invested in efforts into the further development of membrane/diaphragms for water electrolysis systems working to improve their associated ionic conductivities, reduce gas diffusion rates, increase temperature and current density thresholds, and improve lifespan and durability. Many researchers, however, have noted the potential advantages of developing an electrolyser that is capable of operating without the use of these separation structures. If membraneless operation is achieved, it would alleviate the limitations and issues listed above. A membraneless electrolyser would thus easily lend itself to many applications without the need to further develop/innovate the electrolyser’s components. A membraneless electrolyser could potentially operate with a variety of electrolyte types with increased purity tolerances of water feeds. Temperature and pressure conditions of the electrolyser would be dependent on the materials of construction and not based on the limiting conditions set by the membrane or diaphragm structure, as these structures are known to dehydrate, deform and degrade at elevated operating temperatures [77].

With the notable advantages associated with the membraneless approach, researchers have attempted to design and operate a membraneless electrolyser through innovative design philosophies. Two notable alternatives to the membraneless DEFT™ approach are noted below.

### 2.4.1 Baffle Divided Flow/Buoyancy Driven Membraneless Electrolyser

An image of the design/operating principle is provided in Figure 2-9. The electrolyser makes use of flow-through electrodes with a central baffle that separates the anode and cathode. Several journal articles have been published on this design, which focuses on the testing of the device in different configurations (parallel and angled electrodes) with different electrolytic solutions (brine, acid and alkaline solutions) [76], [78], [79].

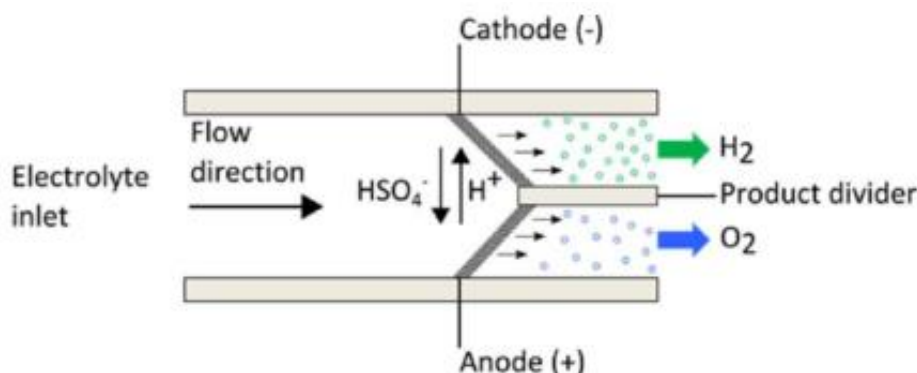


**Figure 2-9: Schematic of an angled electrode baffle divided membraneless electrolyser. (Extracted from [78] – Open Access)**

Performance data was obtained for the operation of the cell, however, the extent of gas separation determinations was based mainly on visual observations with the device manufactured from transparent materials [78], [79]. Adequate gas separations were noted only with the existence of substantial fluid flow rates with flow velocities of  $13.2 \text{ cm.s}^{-1}$  ( $0.132 \text{ m.s}^{-1}$ ) noted to provide a visual indication of appropriate gas separation. Current densities of  $150 - 200 \text{ mA.cm}^{-2}$  at  $2.5 \text{ VDC}$  in  $1.0 \text{ M KOH}$  were observed [78]. The high and variable electrode gap is predicted to be the reason for the poor performance noted. With the variable electrode gap, current density across the electrode is expected to be non-uniform with the highest gas production rates at the point of least efficient separation i.e., the point of lowest electrode gap.

There are, however, some notable advantages associated with this technology. The design allows for buoyancy-driven gas separation with the possibility of upscaling the technology. Scaling, however, would occur at higher electrode gaps and hence large ohmic losses. The inventors have theorised installing this technology on floating photovoltaic (PV) arrays to be deployed in seawater where efficiency losses may be warranted due to available space and the low cost of power input. This design may be advantageous in this sense due to the few components needed for its operations and its potential ability to scale [79]. Demonstrations have, however, not extended past lab-scale prototypes [76], [78], [79].

## 2.4.2 Laminar Flow Membraneless Electrolysis

An image of the design/operating principle is provided in Figure 2-10. This approach to membraneless operation tries to make use of fluid flow patterns to effectively separate the produced gases. This principle makes use of laminar flow and is reliant on the Serge-Silberberg effect. This describes the phenomena where the flow pattern across the flow channels results in a net inertial force on the gas bubble produced that forces them against the wall of the device [80].

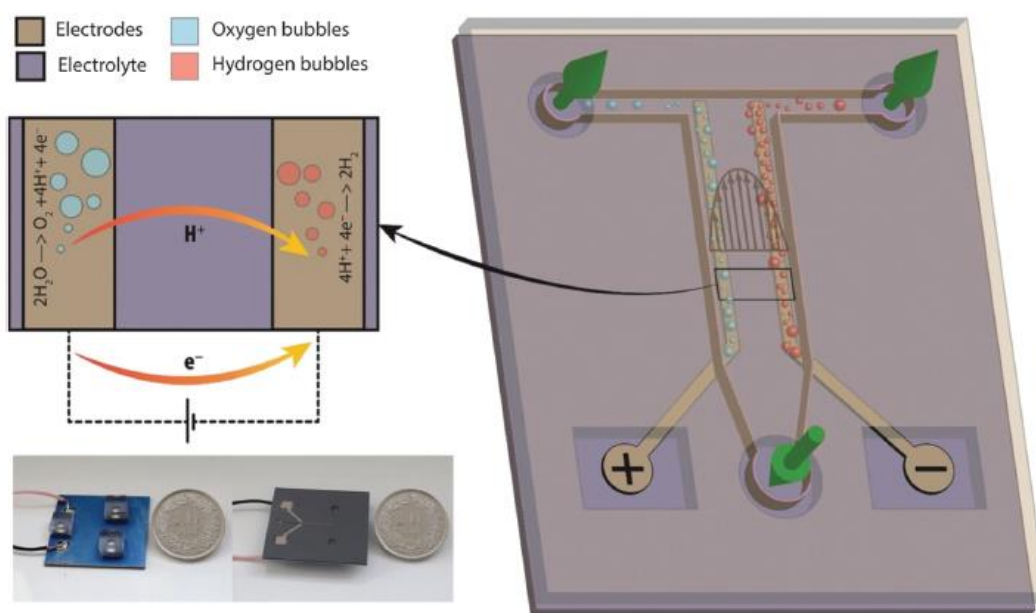


**Figure 2-10: Schematic of laminar flow-based membraneless electrolyser. (Extracted from [80] - Permission Granted in Appendix G)**

Effective gas separation was visually noted at flow rates of  $10 \text{ ml.hr}^{-1}$ . At this flowrate current densities of  $250 - 350 \text{ mA.cm}^{-2}$  were noted at 2.5 VDC in a 1.0 M KOH solution [80]. This operating concept was, however, only tested at the micro-scale and has limited potential to scale to industrial outputs, with the inventors of the technology planning on scaling through the development of multiple devices into a stacked array [80].

## 2.5 Catalysts in Liquid Alkaline Electrolysers

As noted in Section 2.1.2, in a well-designed electrolytic cell the activation overpotential, better known as reaction overpotential, can be considered to be one of the largest contributors to the overall cell overpotential. The reaction overpotential can be reduced with the use of

electrocatalysts that provide an alternative reaction pathway to lower the activation energy. The reaction rate, and hence the current density, at a specified voltage, is dictated by the reaction kinetics of the electrocatalyst. The four-electron oxidation of water (OER) has slow reaction kinetics, thus requiring a large overpotential at specified current densities, and hence limiting the overall efficiency of the electrolysis unit [51]. For this reason, the development of an inexpensive, stable, and effective anodic electrocatalyst has been the topic for numerous studies.

It is well established that platinum group metals such as platinum, iridium and ruthenium exhibit high catalytic activity in acidic environments (i.e. PEM systems) [20], [25], however, these elements are found in low abundance on earth, and thus their use comes at a high cost. Further to this, this high activity does not necessarily carry over to alkaline environments and some elements, such ruthenium, are known to suffer from deactivation through dissociation in both acidic and alkali media [81]. Studies have shown,  $\text{IrO}_2$  exhibits high activity to the OER in both acidic and alkali media, however, several inconsistencies have recently appeared in published findings showing the activity of thin-film transition metal oxides/oxyhydroxides in alkali media to be higher than that seen for PGM electrocatalyst [82]. Figure 2-11 shows a Tafel plot by Trotochaud *et al.* indicating the overpotential seen over a range of current densities for a thin film of 2 – 3 nm thick in a solution of 1 M KOH [82].

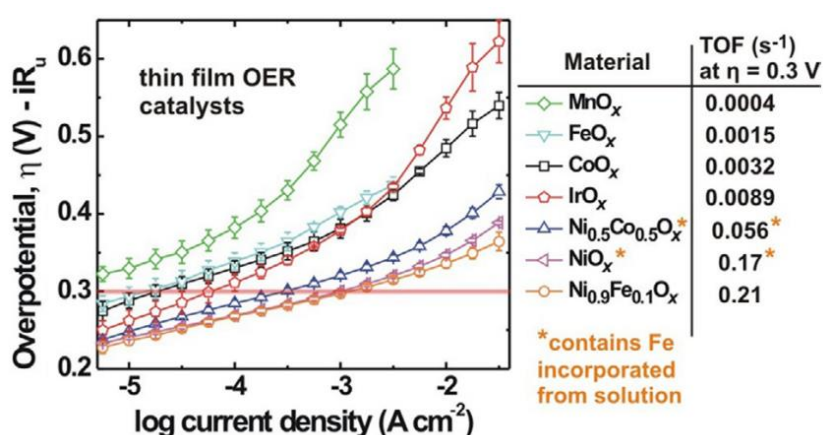


**Figure 2-11: Tafel plot of metal oxides of 2-3 nm thick in a 1M KOH solution**

**(Extracted from [82] – Permission Granted in Appendix G)**

The  $\text{IrO}_2$  electrocatalyst shows high efficiencies at low current densities, however, the Tafel slope is seen to increase rapidly showing low efficiencies at higher current densities.  $\text{IrO}_2$  is expected to show high efficiencies in lab-scale testing, however, it would demonstrate high overpotentials at the operating current densities of commercial electrolyzers. At higher current densities, the nickel oxide and nickel-iron oxide both show low overpotentials and higher turnover frequencies, with nickel-iron oxide showing the best overall efficiency. The study indicates that doping the

nickel oxide matrix with Fe improves the activity of the electrocatalyst for the OER. Cheng *et al.* predicted that the activity for the OER, of the transition-metal oxides/oxyhydroxides, is related to the metal hydroxide bond strength (M-OH), indicating the order of activity as being Ni < Co < Fe < Mn [83].

The iron oxide/oxyhydroxide having a strong Fe-OH bond, acts as an active reaction site working to lengthen/weaken the oxygen-hydrogen bonds, therefore, reducing the activation energy for reaction. It is important to note that, studies showing high activities for the OER utilising transition-metal oxides/oxyhydroxides do so for thin films. Metal oxides, such as iron oxide, are very poor conductors with Table 2-5 showing the conductivity, measured at 20°C, for various metals and metal oxides.

**Table 2-5: Metal and metal oxide conductivities at 20 °C**

| Material  | $\sigma$ at 20 °C (S/m) | Ref  | Material                       | $\sigma$ at 20 °C (S/m) | Ref  |
|-----------|-------------------------|------|--------------------------------|-------------------------|------|
| Copper    | $5.98 \times 10^7$      | [84] | Iron                           | $1.04 \times 10^7$      | [84] |
| Gold      | $4.52 \times 10^7$      | [84] | Platinum                       | $9.44 \times 10^6$      | [84] |
| Aluminium | $3.5 \times 10^7$       | [84] | Fe <sub>4</sub> O <sub>3</sub> | $10^2 - 10^3$           | [85] |
| Tungsten  | $1.82 \times 10^7$      | [84] | NiO                            | $1.3 \times 10^{-3}$    | [86] |
| Nickel    | $1.46 \times 10^7$      | [84] | Fe <sub>2</sub> O <sub>3</sub> | $10^{-7} - 10^{-10}$    | [87] |

Due to the poor conductivity of the transition metal oxide/oxyhydroxide, the composition and thickness of the oxide film has a direct link to the activity of the electrocatalyst. The thin film of metal oxide plated on the substrate introduces superior reaction sites with low activation/reaction overpotentials, increasing the overall surface area of the electrode and minimising the loss of activity due to conductivity limitations. These thin-film catalysts do, however, have a limited lifespan. Selecting the desired thickness of the transition metal oxide/oxyhydroxide film can be regarded as a trade-off between the activity and lifespan of the electrocatalyst. Due to the low conductivity of the transition metal oxides/oxyhydroxides, the film thickness plated on the substrate is normally limited to the micrometre range. Zou *et al.* determined the correlation between mass loading and the activity of the catalyst on different substrates as shown in Figure 2-12 [88].

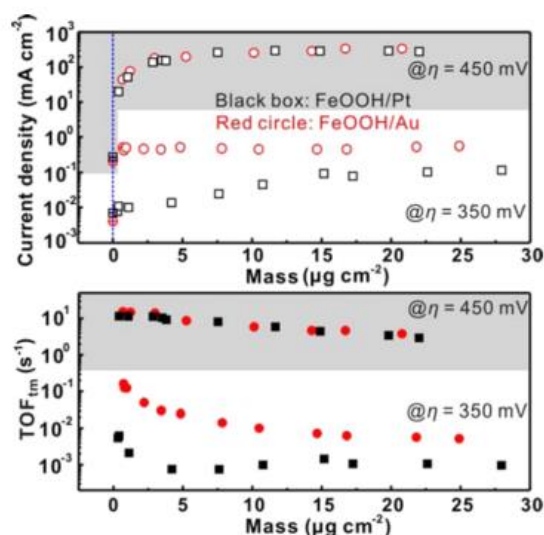


**Figure 2-12: Steady-state current density and TOF for FeOOH on Pt and Au substrate at an overpotential of 350 and 450 mv (Extracted from [88] – Permission Granted in Appendix G)**

The turnover frequency (TOF) refers to the number of catalytic cycles performed by an active site per second. The TOF for an electrocatalyst for the OER can be interpreted as the number of  $O_2$  molecules evolved at an active site per second. From Figure 2-12, it is important to note that the TOF is an intrinsic property of the electrocatalyst allowing for its use as a parameter to assess the activity of the catalyst. Figure 2-12 shows that at an overpotential of 450 mv the current density increases with mass loading up until a value of around  $10 \mu\text{g}/\text{m}^2$ , where the current density is seen to stabilise at a constant value. This result indicates that the FeOOH constituents in the catalyst matrix act as active reaction sites. Beyond the mass loading value of  $10 \mu\text{g}/\text{m}^2$  the addition of excess iron to the catalyst matrix no longer benefits an increase in the current density. This could be due to conductivity limitations, or due to the “overcrowding” of reaction sites in which intermolecular forces result in neighbouring reaction sites becoming temporarily inactive. Further to this, the formation of oxygen gas bubbles at an active site could hinder/block the water molecules from interacting with a neighbouring active site. Depictions of these theories can be seen in Figure 2-13. This theory is supported by the fact that the TOF is seen to decrease with increasing mass loading. In summary, this (Figure 2-12) indicates that there exists a limit where the introduction of reaction sites to the catalyst no longer affects the activity due to the reduction in the TOF of active sites.

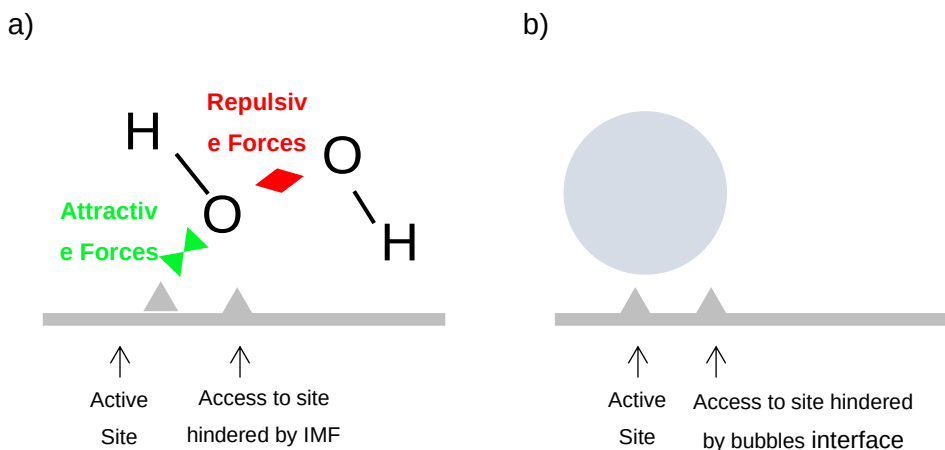


**Figure 2-13: Hindrance theories for decreased TOF at higher % Fe compositions. a) hindrance by intermolecular forces, b) hindrance from bubbles interface.**

Figure 2-14 shows, by comparing the results at an overpotential of 350 and 450 mV, that the substrate can affect the activity of the catalyst film. The results demonstrated that the activity of the catalyst is largely dependent on the substrate material at low overpotential, and relatively independent of the substrate material at higher overpotentials. *Zou et al.* extended their research to investigate the choice of substrate material in the development of the FeOOH catalyst. The results are displayed in Figure 2-14 [88]

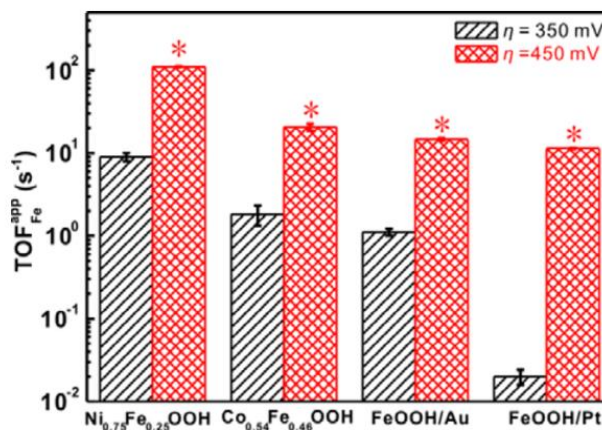


**Figure 2-14: Substrate material dependence on the activity of FeOOH for various metals at 350 and 450 mV (Extracted from [88] – Permission Granted in Appendix G)**

As predicted, the activity is largely dependent on substrate choice at low overpotentials. This dependence starts to diminish at 450 mV. At both overpotentials of 350 and 450 mV the nickel substrate provided increased activity compared to the gold, platinum, and cobalt substrates. The increased activity may be due to the incorporation of nickel molecules into the catalyst film, which works to improve conductivity and provides additional reaction sites.

With the case of the transition metal oxides/oxyhydroxides, in which molecules from the substrate may be incorporated into the matrix of the catalyst film, the activity of the electrocatalyst is largely dependent on the composition (%Fe) of the catalyst film. The introduction of FeOOH based reaction sites work to improve the activity of the catalyst, however, its poor conductivity can negatively affect the rate of electron transfer. Cheng *et al.* investigated the impact of the Fe composition of the catalyst layer on the activity of the catalyst towards the OER [83].

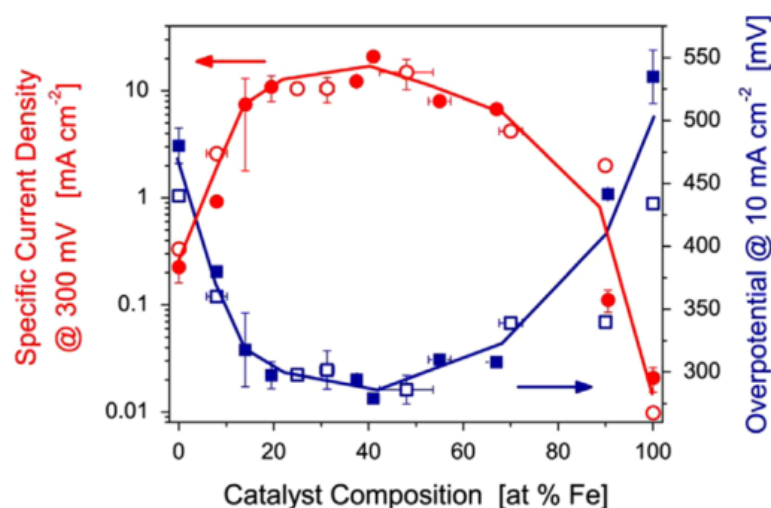


**Figure 2-15: The impact of catalyst composition (%Fe) on the catalytic activity in 0.1 M KOH and a film thickness of 75 nm on nickel support (Extracted from [83] – Open Access)**

Figure 2-15 shows that the overpotential, to achieve a set current density of  $10 \text{ mA}\cdot\text{cm}^{-2}$ , is inversely proportional to the Fe composition of the catalyst film. The slope of this trend decreases overtime where an inflection point is seen at a Fe composition of 40%. Beyond a composition of 40% Fe, the further addition of iron works to decrease the activity of the catalyst, therefore, resulting in the overpotential and the Fe composition having a directly proportional relationship. The desired Fe composition is thus seen in the range of 20% to 50% Fe.

## 2.6 Hydrogen Economics

### 2.6.1 Grey and Blue Hydrogen Economics

There are several methods of producing pure hydrogen currently in industry, of which steam methane reformation (SMR), coal gasification, and water electrolysis are the most common. A large volume of hydrogen is produced in the form of ammonia and methanol, however, further processing is required before pure hydrogen can be obtained. Water electrolysis provides the

most practical means by which green hydrogen can be produced, through the technology's ability to be powered by renewable energy sources, while SMR and coal gasification rely on natural gas, oil and coal reserves to produce both blue and grey hydrogen. Where grey hydrogen refers to hydrogen production through carbon emitting fossil fuel processes and blue hydrogen involves the production of grey hydrogen with the implementation of CCUS processes. The main driving factor for the strong market penetration of fossil fuel-derived hydrogen is the lower associated production costs compared to hydrogen produced by electrolytic means. Figure 2-16 and Figure 2-17 exhibit the cost breakdown, in various geographic locations, for SMR with and without the incorporation of carbon capture, utilization and storage (CCUS) strategies [13] and a market share breakdown for various hydrogen production processes [89].

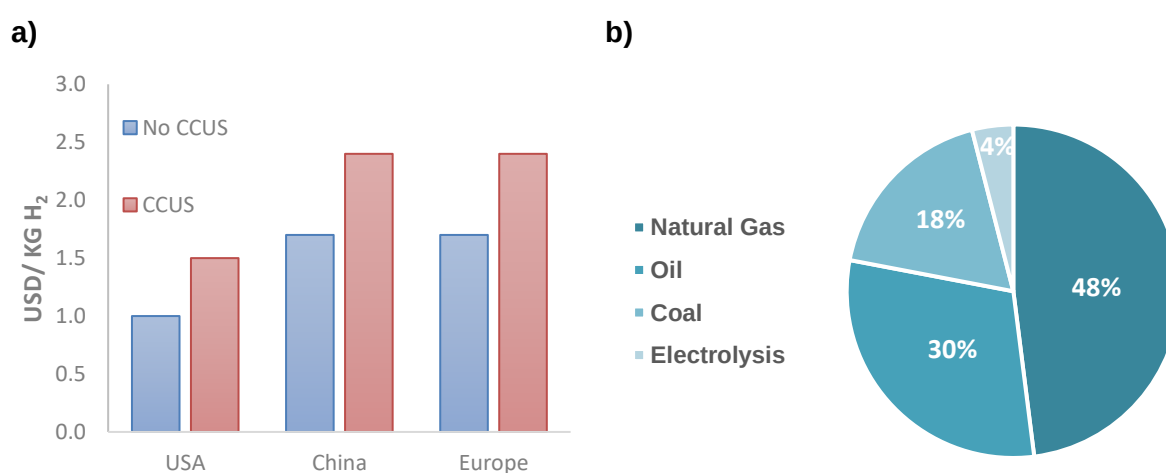


**Figure 2-16: Infographic showing a) Associated costs of hydrogen production with and without the implementation of CCUS processes (adapted from [13]) b) Distribution of hydrogen production methods (adapted from [89]);**

SMR with no carbon capture, utilization and storage (CCUS), is currently the most common hydrogen production method accounting for roughly 48% of global hydrogen production. This is due to low production costs, large processing capacity and the technology maturity level. Figure 2-16a. shows that the cost associated with SMR hydrogen production is dependent on the plant's geological location. Countries with low gas prices, such as the case in the USA, will experience lower feedstock costs hence lower hydrogen production costs. Countries such as China, which are reliant on natural gas imports, will not experience the same favourable economics [13]. Carbon capture is an expensive process and will invariably increase production costs, however, in the case of SMR and coal gasification, it may result in a lower overall hydrogen costs, as carbon taxes are curbed through CCUS. Consequently, whether the hydrogen production cost increases or decreases with the implementation of CCUS processes is dependent on the cost of CO<sub>2</sub>

emissions, i.e., the extent or magnitude of carbon taxes. Once again the CCUS SMR hydrogen production costs are dependent on the policies and carbon penalties of the country of operation [13].

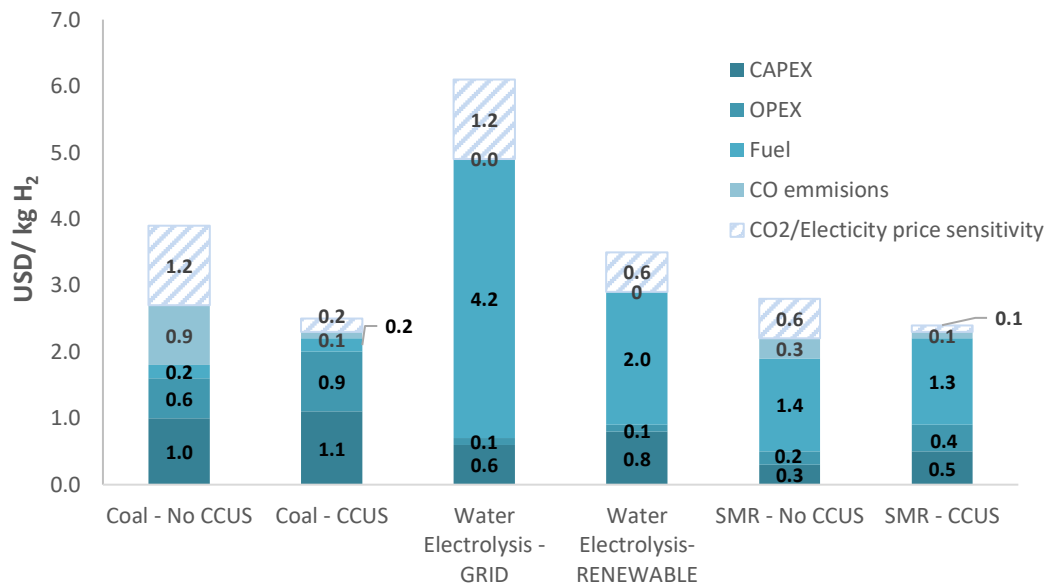


**Figure 2-17: Production cost breakdown for various hydrogen production methods (adapted from [13])**

The cost of grey hydrogen produced from SMR with no CCUS, sensitive to carbon tax penalties, ranges from 2.2 to 2.8 USD/kg H<sub>2</sub>, in comparison 2.7 – 3.9 USD/kg H<sub>2</sub> for hydrogen produced from coal gasification with no CCUS [13]. According to Timmerberg *et al.*, SMR has the lowest CO<sub>2</sub> abatement costs of ~ 27 USD/ton CO<sub>2</sub>, while other hydrogen production methods, such as coal gasification, are > 159 USD/ton CO<sub>2</sub> [90]. For carbon-intensive processes, such as coal gasification, CO<sub>2</sub> rebates can compensate for the cost of CCUS units. Coal gasification has a carbon intensity of ~ 20 kg CO<sub>2</sub>/kg H<sub>2</sub>, while SMR has an intensity of ~8 kg CO<sub>2</sub>/kg H<sub>2</sub> [13]. In such cases, similar production prices for both CCUS SMR and coal gasification processes are realised. The competitiveness of green and blue hydrogen in the foreseeable future is dependent on the price of renewable energy and the price of natural gas with the price of renewable energy having to drop to 10 USD/MWh, at a constant gas price. Higher gas prices would make renewable electricity cost-competitive, such that if the gas price increases to 11 USD/MBtu, renewable electricity for hydrogen production would be competitive at costs ranging from 30-45 USD/MWh depending on electrolyser size and capacity factor [13]. It is important to note that although electrolytic hydrogen production through the grid and renewable power supply represents a cost of 4.9 – 6.1 USD/kg H<sub>2</sub> and 2.9 – 3.5 USD/kg H<sub>2</sub> respectively, the hydrogen produced could be done so on-site thus eliminating the need for costly transportation and logistical channels.

Production of green hydrogen through water electrolysis is becoming the more likely pathway for industry, as renewable electricity prices are predicted to drop even further [91]. As seen in Figure 2-17, both fuel and CAPEX costs contribute significantly towards the production costs for electrolysis hydrogen at 60% and 30% respectively. A further drop in renewable electricity prices would see green hydrogen produced through water electrolysis becoming cost competitive with SMR prices. The cost per kg H<sub>2</sub> in Figure 2-17 applies to the large-scale production of hydrogen [13]. Small-scale production of hydrogen through water electrolysis will be more costly due to the higher CAPEX contribution proportion.

## 2.6.2 Alkaline Water Electrolysis Techno-economics

Currently, when looking at pure production costs, ignoring transportation, distribution and logistics, the cost to produce hydrogen through water electrolysis is the highest of all hydrogen production methods, however, there is still room for the improvement of existing technologies. Several parameters affect the overall cost of hydrogen production for electrolyser technologies, namely, the system CAPEX, OPEX and electrical costs. These parameters are dependent on the system's performance, size, and application. The cost breakdown for general large-scale alkaline systems (forecourt) is provided in Figure 2-18.

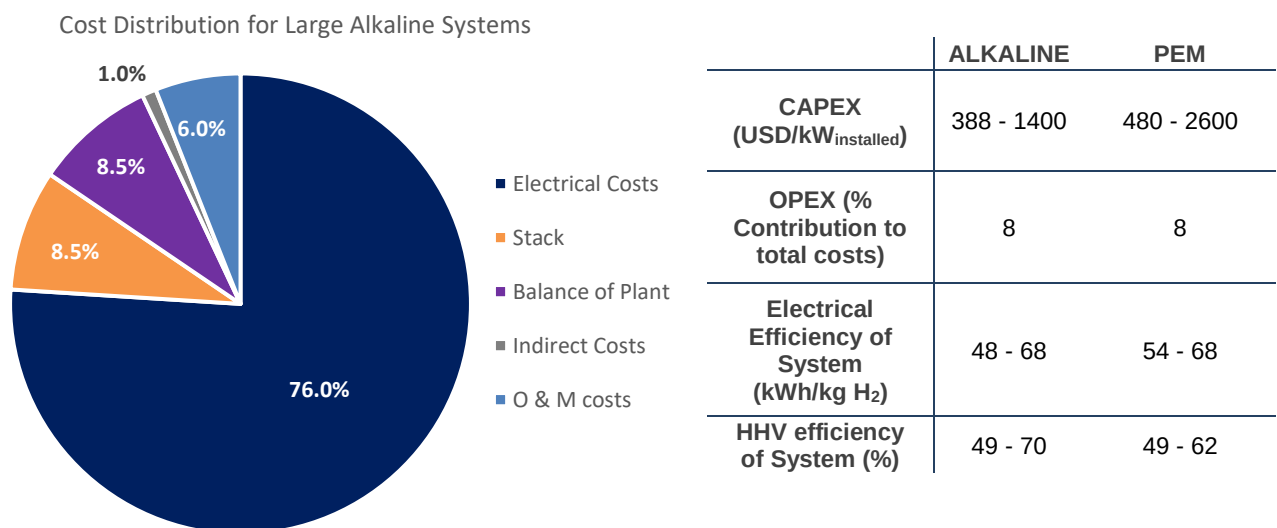


**Figure 2-18: Cost distribution for large alkaline electrolysis systems [18], [92], [93]**

Figure 2-18 shows that CAPEX contributions of large alkaline systems (forecourt) make up approximately 17% of an alkaline electrolysis system's lifespan costs, of which the stack accounts for approximately 50% of the CAPEX contributions, with PEM systems having a higher CAPEX

contribution due to their high manufacturing costs and PGM's being present in the membrane electrode assembly. Operations and Maintenance (O&M) OPEX contributes approximately 6 - 8% to the total costs, while electrical costs contribute as much as 76%. The electrical cost contribution is, however, dependant on the electrical efficiency of a system, definition of the system boundary, and the cost of electricity in the region that the electrolyser system is being operated. These values, however, represent large scale electrolyser systems, with predicted capacities in the MW scale. Large production rates are used as a basis to obtain cost and performance data, as electrolysis systems exhibit the highest technical and economic viability at these scales. Figure 2-19 shows the general cost and performance parameters for small scale alkaline and PEM electrolyzers.

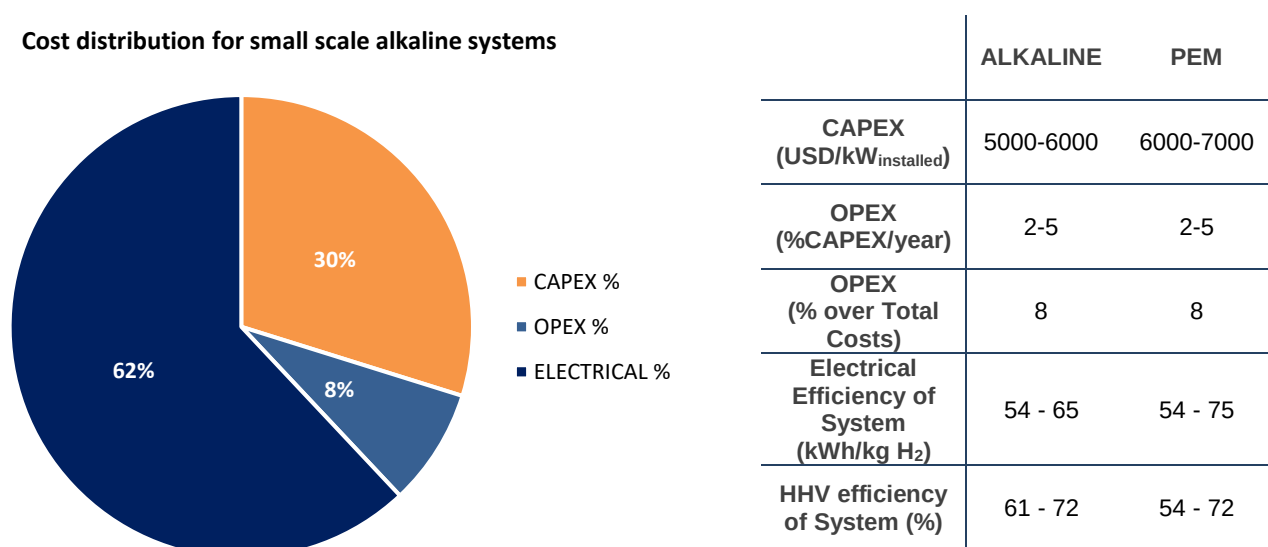


**Figure 2-19: Cost distribution for small scale alkaline electrolysis systems [93], [94]**

Figure 2-19 notes a sharp increase in the CAPEX per kW and a decrease in system efficiencies. This result shows how alkaline electrolysis units are reliant on economies of scale. The large-scale and small-scale systems both require the same degree of instrumentation and other balance of plant (BOP) components. At low scale production, the cost and power consumption of instrumentation and other plant auxiliaries cannot be offset to the same degree as what is possible at higher production outputs.

### 2.6.2.1 Alkaline System CAPEX and OPEX

The CAPEX of electrolysis systems comprises of three major sectional areas, namely the electrolysis stack, the immediate balance of plant costs (BOP) and post-production gas processing. As noted in Figure 2-18, the stack accounts for the largest weighting of the systems CAPEX, therefore, it is important to note the cost contributions of stack components. Figure 2-20 provides a generic cost breakdown for a large forecourt alkaline electrolysis stack [93], [95].

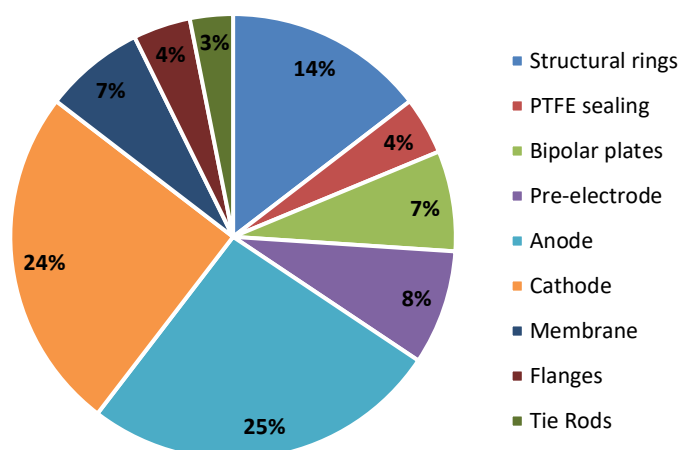


**Figure 2-20: Stack component cost contribution for an alkaline electrolyser (adapted from [93])**

Figure 2-20 shows that the membrane electrode assembly is the largest contributor to stack costs accounting for 64%, with membranes contributing 7% and the anode and cathode contributing 49% to the overall cost of the stack. The high anode and cathode contributions are mainly because electrode material is manufactured from nickel and later coated with a variety of catalyst coatings many of which still include PGM materials. The low current densities in liquid alkaline systems result in large electrode areas being required to meet set production outputs. Cost of cell components (other than the MEA) can be reduced by increasing the electrode area contained in a single cell, however, the electrode area is set by current density and hence contributes largely to the overall cost of the stack. Figure 2-20 provides a representative overview of the cost breakdown of alkaline systems, however, this breakdown may differ depending on the manufacturer's unique operating philosophy. Figure 2-21 shows the BOP cost breakdown for both small and large-scale production:

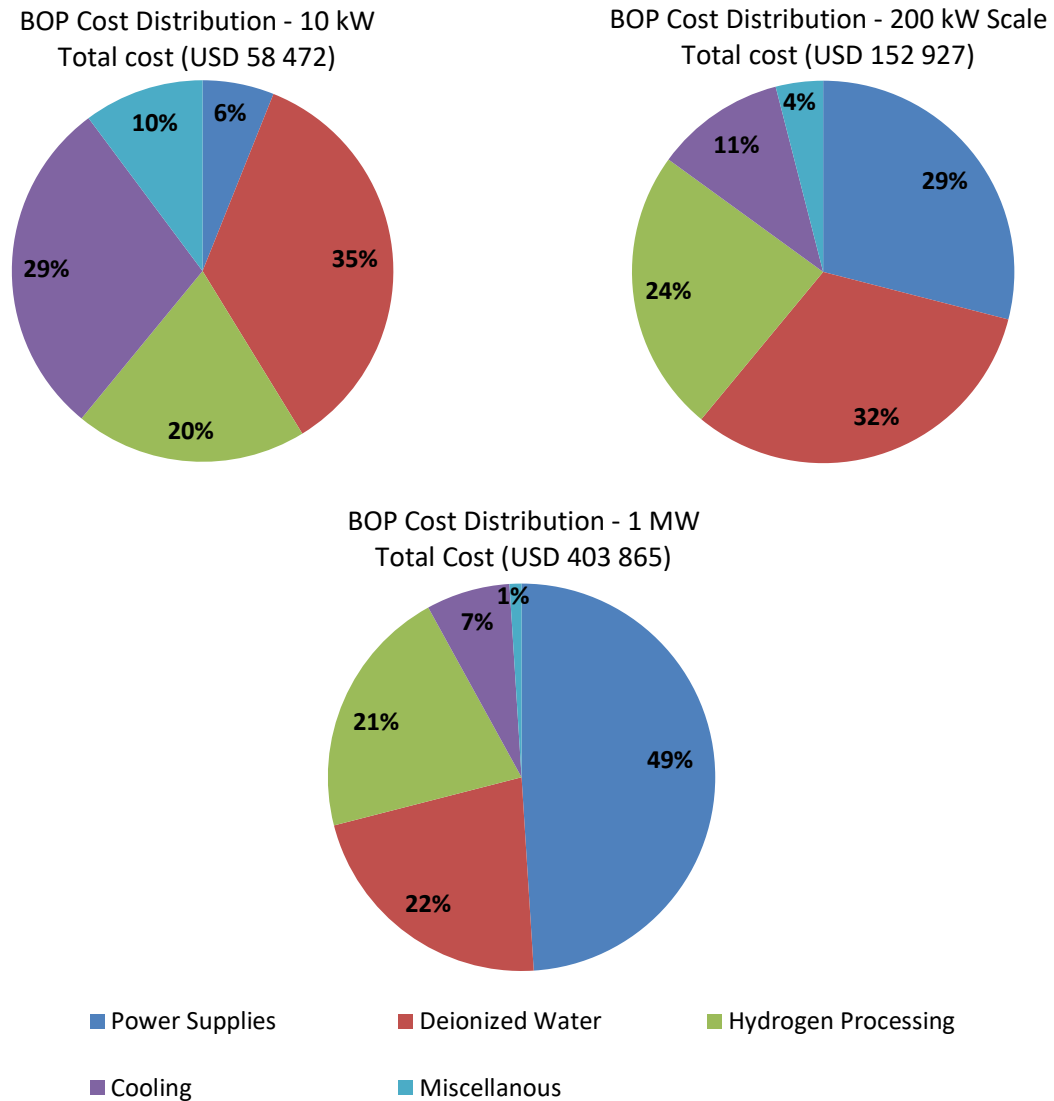


**Figure 2-21: Balance of plant cost breakdown for alkaline systems at various production rates [95], [96].**

Figure 2-21 shows that in the 10 kW range a CAPEX of 5 847 USD/kW<sub>installed</sub> is realised. This is in line with the data provided in Figure 2-19. At a power capacity range of 10 kW, the deionised water generation and feed to the electrolysis plant contributes the greatest cost weighting. The de-ionised water generation system includes feed pumps, cation and anion exchangers, parameter transmitters (flow, temperature, pressure, conductivity), an oxygen separation tank and a water storage vessel [96]. This is followed by the electrolyte cooling system with an estimated 29% cost contribution. Approaching the 200 kW scale the CAPEX estimate is reduced to 765 USD/kW<sub>installed</sub> with the power supply contributing a large factor to the overall cost. At 200 kW production output power conditioning equipment increase in costs due to the need to handle high

current outputs whereas costs of the demineralised and cooling systems can be offset with economies of scale. Moving to the MW scale a CAPEX estimate of 404 USD/kW<sub>installed</sub> is noted, with power conditioning equipment now accounting for almost half of the balance of plant costs. The processing equipment maintains roughly the same cost contribution across the size ranges. This is since the drying and deoxidising beds are specified according to gas production outputs thus cost increases readily with production out.

O&M expenditure for electrolysis systems includes scheduled maintenance, stack & equipment replacements, water & chemical costs, and indirect costs. O&M expenditure does not include electrical costs, as the electrical cost contribution for electrolysis systems is one of the main cost drivers and hence is considered as an individual cost parameter. Table 2-6 provides O&M expenditure industrial benchmarks.

**Table 2-6: Industry benchmarks for O&M costs for small- and large-scale electrolysis units [18], [93], [94], [97]**

| OPEX Value                                                                                                                                                                                   | Large Scale Production | Small Scale Production |
|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|------------------------|------------------------|
| <b>\$/kW/year –</b>                                                                                                                                                                          |                        |                        |
| <ul style="list-style-type: none"> <li>System boundary around the stack</li> <li>Stack replacements are excluded.</li> </ul>                                                                 | 9 – 44                 | 69 - 80                |
| <b>% CAPEX –</b>                                                                                                                                                                             |                        |                        |
| <ul style="list-style-type: none"> <li>Calculated by: (System OPEX per year) / (System CAPEX)</li> <li>System boundary around the stack</li> <li>Stack replacements are excluded.</li> </ul> | 2 – 5 %                | 6 - 13 %               |
| <b>% Total Costs –</b>                                                                                                                                                                       |                        |                        |
| <ul style="list-style-type: none"> <li>Calculated by: (System OPEX) / (Total costs)</li> <li>Includes replacements and full system maintenance.</li> </ul>                                   | ±37%                   | ±60%                   |

### 2.6.2.2 Electrical Costs

The electrical cost contribution of electrolytic systems is the largest contribution to hydrogen production costs. Electrical costs are dependent on two main cost-driving factors: the electrical efficiency of the electrolyser stack and system, and the price of electricity. The electrical efficiency of the stack and system are intrinsic properties of an electrolysis system, and therefore plays a crucial role in determining the market competitiveness of a system. Table 2-7 shows the reported electrical efficiencies of industrial competitors and market studies:

**Table 2-7: Literary and manufacturer system power consumption parameters for the operation of alkaline electrolysis units.**

| Source                    | Energy Consumption<br>(kWh/kg H <sub>2</sub> ) | HHV%    | Ref        |
|---------------------------|------------------------------------------------|---------|------------|
| IEA                       | 48 - 53                                        | 74 - 82 | [13]       |
| IRENA                     | 49 - 51                                        | 77 - 80 | [89]       |
| Bertuccioli <i>et al.</i> | 49 - 67                                        | 59 – 81 | [93]       |
| Nel Hydrogen              | ±50                                            | ±79     | [93]       |
| Hydrogenics               | 55 – 58                                        | 66 - 68 | [93], [98] |
| McPhy                     | 50 - 58                                        | 53 - 79 | [93], [99] |
| Teledyne Energy systems   | 59 - 62                                        | 64 - 67 | [17]       |

Typical industrial and market electrical efficiencies range from 48 to 65 kWh/kg H<sub>2</sub> for both small and large-scale production. An electrical efficiency of 48 kWh/kg hydrogen was reported by Nel Hydrogen and is most likely obtained from large scale systems, however, most small to medium production systems are reported to be within the 55 to 60 kWh/kg hydrogen operating electrical efficiency [19], [20], [59]. Electrical efficiencies of an electrolysis system can be improved through decreasing cell potential by producing larger stacks, or by improving the operating current density per cell. The former can only be achieved at a higher system CAPEX, increasing the overall system costs. Due to this trade-off between system CAPEX and OPEX alkaline systems generally find an optimal operating point (point of lowest hydrogen cost) at the 1.8 – 2 VDC range (48 – 53 kWh/kg H<sub>2</sub>). Consequently, although the below 50 kWh/kg H<sub>2</sub> operating point is possible, voltages below 1.8 VDC ) would be required which implies low current densities and greater CAPEX requirements and hence is not readily seen in industrial application.

The cost of electricity varies geographically and is dependent on the energy source and method of production. The price of electricity will largely determine the electrical costs of an electrolysis system, and so it is important to target lower electricity prices to yield an economically feasible system. Table 2-8 below shows the cost per kWh of electricity for various countries.

**Table 2-8: Electricity Prices for various geographical areas [100]**

| Country     | Price (\$/kWh) | Country      | Price (\$/kWh) |
|-------------|----------------|--------------|----------------|
| Germany     | 0.35           | Norway       | 0.14           |
| Denmark     | 0.34           | US           | 0.14           |
| Italy       | 0.26           | Canada       | 0.11           |
| Australia   | 0.25           | South Africa | 0.11           |
| Netherlands | 0.25           | South Korea  | 0.09           |
| UK          | 0.25           | UAE          | 0.08           |
| France      | 0.19           | China        | 0.08           |
| Brazil      | 0.18           | India        | 0.08           |
| Iceland     | 0.16           | Japan        | 0.29           |

With the high prices associated with grid electricity usage and the ever-reducing costs of renewable power generation, electrolytic hydrogen production has found potential to become cost-competitive or even carry a cost advantage with linkage to low-cost renewable power. Studies conducted by IRENA show that renewable energy costs have been significantly dropping and consequently, have started to become competitive, and in some cases, cheaper than grid-supplied electricity. Table 2-9 is taken from the IRENA renewable energy datafile and shows the drop in renewable energy prices from 2010 to 2018 [100].

**Table 2-9: Renewable energy power generation costs for 2010 and 2019 [100]**

| Renewable Energy Source  | 2010 (\$/kWh) | 2019 (\$/kWh) | % Change |
|--------------------------|---------------|---------------|----------|
| Bioenergy                | 0.076         | 0.066         | 13%      |
| Geothermal               | 0.049         | 0.073         | 49%      |
| Hydroelectric            | 0.037         | 0.047         | 27%      |
| Solar Photovoltaic       | 0.37          | 0.068         | 82%      |
| Concentrated Solar Power | 0.346         | 0.182         | 47%      |
| Offshore wind            | 0.161         | 0.115         | 29%      |
| Onshore wind             | 0.086         | 0.053         | 38%      |

Table 2-9 shows a significant drop in prices for photovoltaics and wind energy over the past decade, however, hydroelectric, and onshore wind energy still proves to be the cheapest option for electricity. Solar photovoltaics exhibit the largest price drop and are the most popular renewable energy option due to the simplicity and low cost associated with their setup, however, linking solar power to alkaline electrolysis systems brings about associated issues. The first being the intermittent nature of solar power and the effects this has on alkaline electrolysis as discussed in Section 2.2. The second being the fact that solar power production is limited to a nominal period of 6 - 7 hours of energy generation. This severely reduced capacity factor harms the overall cost to produce hydrogen. Although the input power results in a reduction in electrical OPEX, the CAPEX of the plant is only offset by roughly a quarter of that for 24-hour hydrogen production as the amortisation period remains the same, yet, the system only produces hydrogen over a portion of that period.

### **2.6.2.3 Post Gas Production Costs**

The preparation of hydrogen includes the purification, compression/pumping, storage and ultimately distribution/dispensing of hydrogen product to the specifications required by the specific application. The contributing cost factors towards the preparation of the hydrogen product include the installation costs of compressing and pumping, purification, and storage systems, as well as the operating costs associated with the above-mentioned units. The extent of preparation is determined by the type of transportation, the form, and the end-use of the product. The cost of preparation for transporting gaseous hydrogen through truck and pipeline is approximately 0.8 and 0.3 USD/kg H<sub>2</sub> respectively, while the transportation of liquid hydrogen (pure), is approximately 1.6 USD/kg H<sub>2</sub> [12]. This is followed by further distribution and carrying costs with estimates of 1.0 and 1.6 USD/kg H<sub>2</sub> for the gaseous trucking and piping respectively and 0.4 USD/kg H<sub>2</sub> for distribution of liquid hydrogen [12], [13]. The costs provided are dependent on the distance of transmission, however, the costs offer a good estimate for local distribution < 500 km.

According to the California Fuel Cell Partnership, the current price of hydrogen from the nozzle ranges between 13 to 16 USD/kg H<sub>2</sub>, which leaves hydrogen at approximately 4 – 6 times more costly than a gallon of gasoline (based on an energy equivalent), however, production costs of hydrogen currently range between 2.5 – 6 USD/kg H<sub>2</sub>, meaning that the transportation and distribution costs account for approximately 55 - 85% of total hydrogen costs. It is therefore important to identify the cost factors in transporting and distributing hydrogen in order to properly assess the end-use cost of hydrogen for both centralised and decentralised production methods. In doing so the cost savings for decentralised electrolytic hydrogen can be assessed and appreciated as the distribution and accessibility of hydrogen gas and will ultimately affect the level

to which hydrogen will integrate into the global market and economy. Although onsite production and consumption of hydrogen would be ideal, as no distribution costs will be incurred, large scale applications and inter-continental trade will require a range of storage and distribution methods. The overall costs within the hydrogen value chain are provided in Figure 2-22.

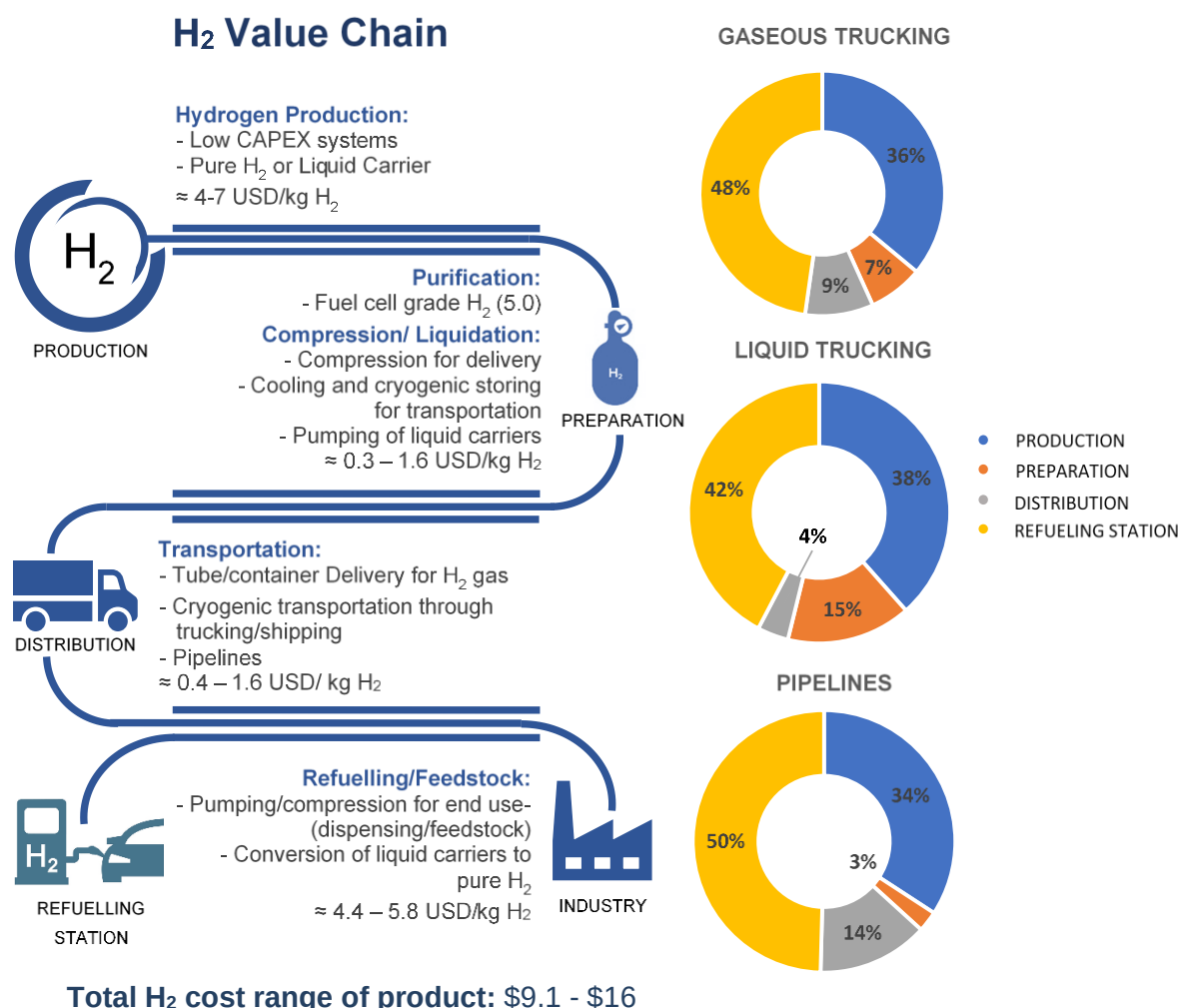


**Figure 2-22: Hydrogen fuel value chain [12], [13], [16].**

#### 2.6.2.4 Analysis of Small Scale Industrial Alkaline Systems

To gain a realistic perspective on the operational and capital costs of small water electrolysis systems, investigations were carried out into several projects using small scale alkaline and PEM electrolyser systems. Cost data for industrial electrolyser systems are not readily available, as many industrial manufactures hold this information as proprietary. Access to this data is usually made available through techno-economic analyses, market reviews or research papers, in conjunction with predicted electrolyser system costs. These sources do not, however, provide

explicit information on small electrolyser systems, but rather provide a general overview of electrolyser system costs, largely based on bigger capacity units. Therefore, small scale water electrolysis projects were used to extract data to provide a reliable comparison for the DEFT™ unit.

**Table 2-10: Techno-economic specifications of various use cases of small scale alkaline and PEM systems**

| Use Case                   | Units                   | Hydrogenics [94]                     | Rome Study [33] | Korea Study [15] | Norway study [101]                  | PERIC (*Quotation) | CEMAC Study [96] |
|----------------------------|-------------------------|--------------------------------------|-----------------|------------------|-------------------------------------|--------------------|------------------|
| <b>Capacity</b>            | (Nm <sup>3</sup> /h)    | 60                                   | 30              | 30               | 30                                  | 2,5                |                  |
|                            | (kg/24 hr)              | 130                                  | 65              | 65               | 60                                  | 5                  | 20               |
| <b>Lifespan of Plant</b>   | (years)                 | 7                                    | 10              | 8                | 10                                  | 7                  |                  |
|                            | (Hours)                 | 60 000                               | 87600           | 70 895           | 90 000                              |                    |                  |
| <b>Electrical Power</b>    | (kW)                    | 312                                  | 156             | 210              | 178,2                               |                    | 10 kW            |
| <b>Efficiency</b>          | (kWh/Nm <sup>3</sup> )  | 5,2                                  | 5,2             | 7                | 5,94                                |                    |                  |
|                            | (kWh/kg)                | 57,8                                 | 58              | 77,8             | 66                                  |                    |                  |
| <b>Lifetime Production</b> | (ton)                   | 324                                  | 236.5           | 189.22           | 120                                 |                    |                  |
| <b>Lifetime MWh used</b>   |                         | 18 720                               | 13 666          | 14 717           | 7 920                               |                    |                  |
| <b>CAPEX</b>               | (\$-Lifetime)           | 630 240                              | 630 240         | 708 950          | 514 471                             | 63 200             | 58 472           |
|                            | (\$/kW <sub>i</sub> )   | 2020                                 | 4040            | 3376             | 2 887                               | 5056               |                  |
|                            | (\$/kg H <sub>2</sub> ) | 1,95                                 | 2,66            | 3,7              | 4,3                                 | 4,95               |                  |
| <b>OPEX</b>                | (\$-Lifetime)           | 172 66                               | 43 136          | 241 830          | 20 579                              |                    |                  |
|                            | (\$/kW <sub>i</sub> )   | 553,42                               | 276,51          | 1151,60          | 115,48                              |                    |                  |
|                            | (\$/kg H <sub>2</sub> ) | 0,53                                 | 0,18            | 1,3              | 0,2                                 |                    |                  |
| <b>Electrical Cost</b>     | (\$-Lifetime)           |                                      | 1 038 730       | 501 420          |                                     |                    |                  |
| <b>Electrical Costs</b>    | (\$/kg H <sub>2</sub> ) |                                      | 4,39            | 2,6              |                                     |                    |                  |
| <b>Overall cost per kg</b> | <b>(\$/kg)</b>          | 2,48 +<br>(C <sub>Electrical</sub> ) | 7,23            | 7,8              | 4,5 +<br>(C <sub>Electrical</sub> ) |                    |                  |

Small scale electrolysis systems were modelled in the above-mentioned use cases, where techno-economic analyses were conducted to investigate the economic feasibility of small-scale electrolysis systems. Detailed information regarding the operating conditions and assumptions

associated with the use cases mentioned in Table 2-10 is provided in Appendix A of this report. Table 17 below summarises the observed technical parameters for small scale electrolysis use cases.

**Table 2-11: Summary of techno-economic parameters for small-scale industrial use cases.**

| Capacity<br>(Nm <sup>3</sup> /hr) | CAPEX<br>(\$/kW <sub>i</sub> ) | OPEX<br>(\$/kW <sub>i</sub> ) | CAPEX<br>(\$/kg H <sub>2</sub> ) | OPEX<br>(\$/kg H <sub>2</sub> ) | \$/kg H <sub>2</sub>                 | Efficiency<br>(kWh/Nm <sup>3</sup> ) |
|-----------------------------------|--------------------------------|-------------------------------|----------------------------------|---------------------------------|--------------------------------------|--------------------------------------|
| 2.5 – 60                          | 5056 - 2887                    | 1151 – 115                    | 4,95 – 2,66                      | 1.3 – 0.8                       | ~ 7,5 including<br>electrical costs. | 7 – 5,2                              |

## 2.7 Section Relevance Summary

As noted in Section 1.4, the study aims to assess scalability, performance, and economic viability of the DEFT™ concept through design modifications followed by prototype demonstration. The main objective is to generate performance and economic data for this assessment from a demonstration of a system that is representative of a realistic small scale industrial solution. The literature review focussed on collecting information to build upon existing work done to optimise the performance liquid alkaline system and to identify variables and parameters that have a presiding effect over the performance of these alkaline systems. Furthermore, identify performance benchmarks for literature provided a means of comparison to current technology offerings.

It was noted that the performance (current density exhibited at set voltages) was heavily dependent operating temperature of the electrolyser stack. Increasing the operating temperature allowed for better utilisation of heat and thus decreased the require electrical input to the electrolyser stack. Furthermore, the conductivity of the liquid electrolyte increases with temperature, therefore, reducing cell ohmic resistances. With conventional membrane/diaphragms being temperature limited, a membraneless DEFT™ electrolyser stack has the unique potential of capitalising on medium temperature (150 – 250 °C). Although this potential in noted it is outside the scope of this study with planned operation of the 3 -5 kg/day H<sub>2</sub> system to occur at atmospheric pressure. A temperature of 80°C will thus form the basis of this assessment as to prevent vaporisation of the liquid electrolyte and to provide a like for like comparison to conventional units which operate at this point. At this temperature, an electrolyte concentration of 30 wt% was noted to maximise conductivity.

It was noted that the thickness of the electrode gap had a large effect on the associated resistance of the cell. Minimising the electrode gap would work to reduce the distance of ionic pathways and

provide better bubble management within the cell (i.e. minimising the electrode gap “bubble curtain”). Furthermore, the system would benefit by moving from a unipolar to bipolar configuration to reduce the amperage requirements of the power condition equipment and to encourage the design and construction of a compact cell design which allows for better control of the electrode gap.

The cathodic and anodic overpotential was noted to carry a large contribution towards the overall cells overpotential, therefore, the successful incorporation of such would work to greatly improve the performance of the electrolyser stack. The development potential was noted within the area, in particular, focusing on transitional metal coatings, however, with the vast variety of catalyst options, this study will focus on performance assessment utilising the common nickel substrate materials as a means of attaining like for like comparisons to conventional technologies removing the performance of the catalyst as a variable.

Lastly, performance and economic data are provided for both fossil fuel derived hydrogen and electrolytic hydrogen production. It is noted that fossil fuels derived hydrogen production methods provides the lowest generation cost, with costs as low as 1 – 2 USD/kg H<sub>2</sub>, however, with the implementation of carbon taxes and/or CCUS technologies these costs approach the price point of 3 – 5 USD/kg H<sub>2</sub> which is comparable to the cost of electrolytic hydrogen generation from low cost renewable energy sources. Furthermore, the generation of fossil fuel derived hydrogen is centralised presenting distribution and logistics challenges with the cost for preparation and transportation ranging from 0.7 to 3.2 USD/kg H<sub>2</sub>. Small scale electrolytic systems were noted to exhibit CAEPX cost ranging from 5000 – 6000 USD/kW<sub>installed</sub> with energy consumption values ranging 54 - 65 kWh/kg H<sub>2</sub>.

## CHAPTER 3 - EARLY DEMONSTRATION PROTOTYPE

### 3.1 Overview

The investigative process for a Divergent Electrode-Flow-Through (DEFT™) alkaline electrolyser, to achieve Hydrox Holdings objectives (listed below), was undertaken for phase 1 of the project:

- Provision for a stack design that permits the scalability of the DEFT™ concept to allow for potential production outputs beyond small scale hydrogen production.
- Together with the enhanced scalability, the design must utilise minimal components with the largest electrode diameter possible to reduce the CAPEX and footprint of the finalised stack.
- The finalised stack configuration must generate gas purities of > 99.5 vol%. for both hydrogen and oxygen.
- The acceptable flow velocities must deliver high purity gas but contribute low parasitic loads to ensure an overall energy consumption of lower than 90 kWh/kg H<sub>2</sub> at a parasitic load of lower than 35% of the overall energy consumption of the plant.

Upon completion of the above-listed objectives, the refinement of a compact, low CAPEX, scalable and reliable reactor would have been realised, with the MCFP stack design forming the basis from which design modifications were implemented. Attention was been paid to increasing the electrode area (electrode flow path) through design changes to the design of the electrodes and changing the way electrolytic fluid is introduced to the electrode. Further to this, the aim was to improve flux distribution employing a meshed structure to increase backpressure and enhance flow velocities between the electrode gap and the electrode itself. The effect of the design modifications to the MCFP stack was assessed through the development of a small-scale prototype and subsequent balance of plant test rig. The following diagram, Figure 3-1, provides a graphical overview of the path taken in developing a scalable reactor prototype for the DEFT™ reactor to take forward:

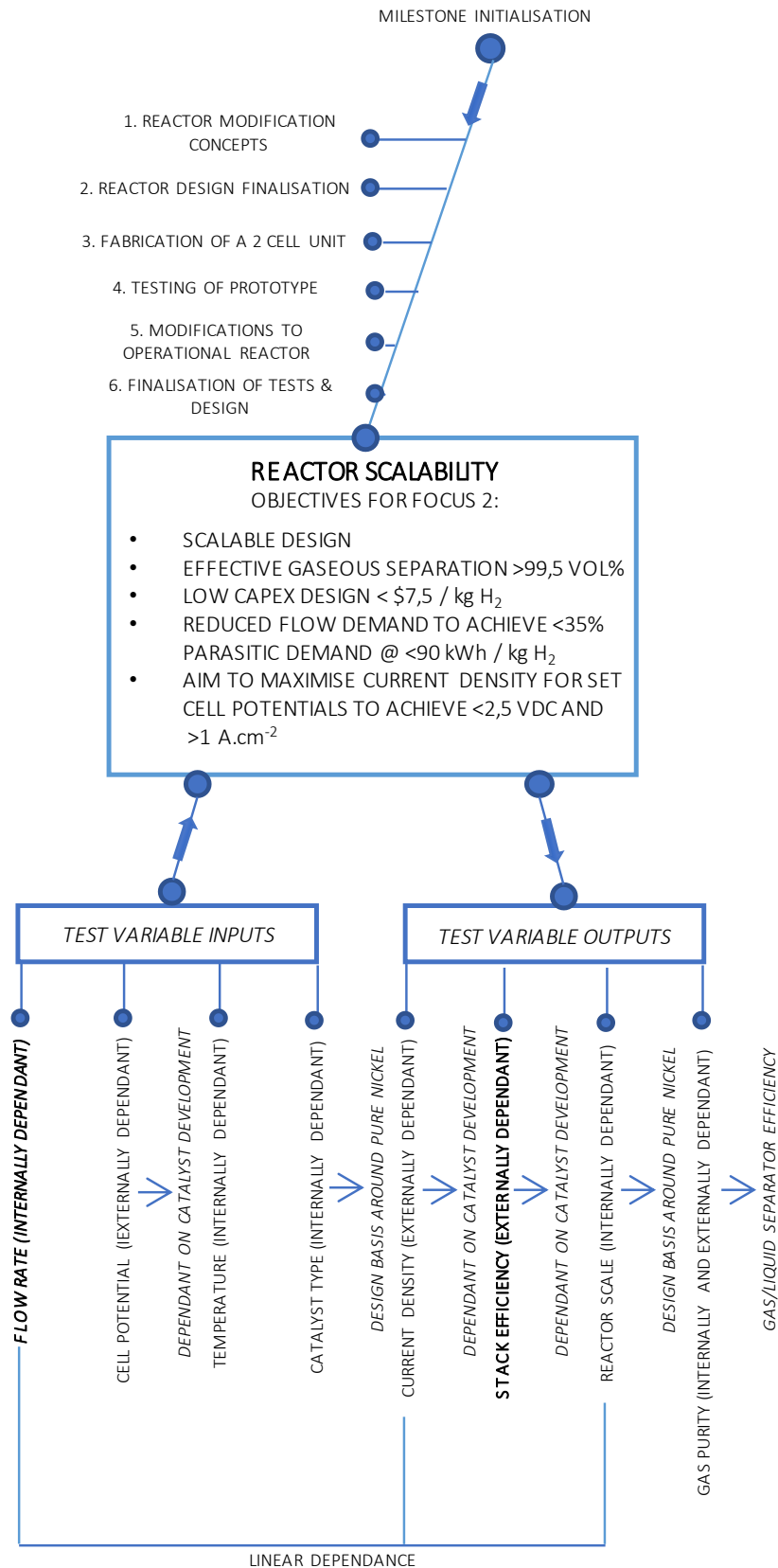


**Figure 3-1: Workflow path for the development of a scalable reactor pathway for the DEFT™ principle**

## Synopsis on inputs

- **Flow rate** – a critical parameter that has a major influence on gas separation based on electrolytic solution properties, gas evolution rates (indirectly the current density), electrode configuration, electrode gap and the solution flow path.
- **Cell potential** – representative of the overpotential of the reactor dependant on numerous parameters such as the desired current density, electrolytic solution properties, electrode gap, electrode configuration, flow velocity and reaction kinetics.
- **Temperature** – has no dependence on other critical parameters, however, the parameter is instrumental on dictating separation efficiency (both within the reactor and separation system) and reaction kinetics.
- **Catalyst type** – the design of the end reactor will be based on a pure nickel surface; however, the development of this parameter will form an external investigation.

## Synopsis on outputs

- **Current density** – an output based on the driving force magnitude to overcome cell resistances and reaction kinetics. The desired trend would be to maximise the current density whilst simultaneously minimising the cell potential.
- **Stack efficiency** – based solely on the selected cell potential operating point above that of the thermal neutral cell potential. It has a lesser dependence on the operating temperature and is noted to not vary to any appreciable extent below 100°C.
- **Reactor Scale** – the chosen configuration coupled to the variation of experimental input ranges will dictate the scale possible for the reactor based on electrode size and flow path length at a constant electrode gap.
- **Gas Purity** – will be dictated by the gas crossover occurring within the reactor, intrinsically dependant on the flow velocity and properties of the electrolytic solution.

## 3.2 Methods and Apparatus

### 3.2.1 Design Modifications from the MCFP Prototype

Numerous challenges were solved through the initial R&D of the MCFP design, however, additional challenges remain so as to allow the DEFT™ technology to be scaled to large hydrogen production outputs while achieving reasonable system efficiencies. To accomplish this, the gaseous production rate was optimised referenced to the reactor footprint along with an order of

magnitude reduction in the required flow velocity for effective gaseous separation. This was achieved by:

- allowing for a greater geometric surface area per electrode,
- electrode gap reduction,
- taking cognisance that catalytic qualities of each electrode could be enhanced, and
- improving on the optimal design parameters established in research and development to date.

#### **3.2.1.1 Annular Electrode Design**

A limit exists concerning the number of porous electrode layers that can be added to a pole pair before performance enhancements become limited showing negligible improvements and before incurring additional OPEX with no real improvement in performance. The alternative to enhancing the geometric area was to enhance the cross-sectional area of the electrode. This could be done in two manners: by allowing for more electrode area or by enhancing the surface characteristics of the electrode to account for more surface specific area. It was initially imperative for the flow path to be limited to the maximum optimal flow path of 15 mm found at an optimal cross-sectional flow velocity of  $0.075 \text{ m.s}^{-1}$  when considering the design for the MCFP prototype reactor. To solve this dilemma, a central annular injection was introduced to produce flow peripherally both from the inside and the outside of the electrode, as a means of providing additional electrode area for a single electrode pair:

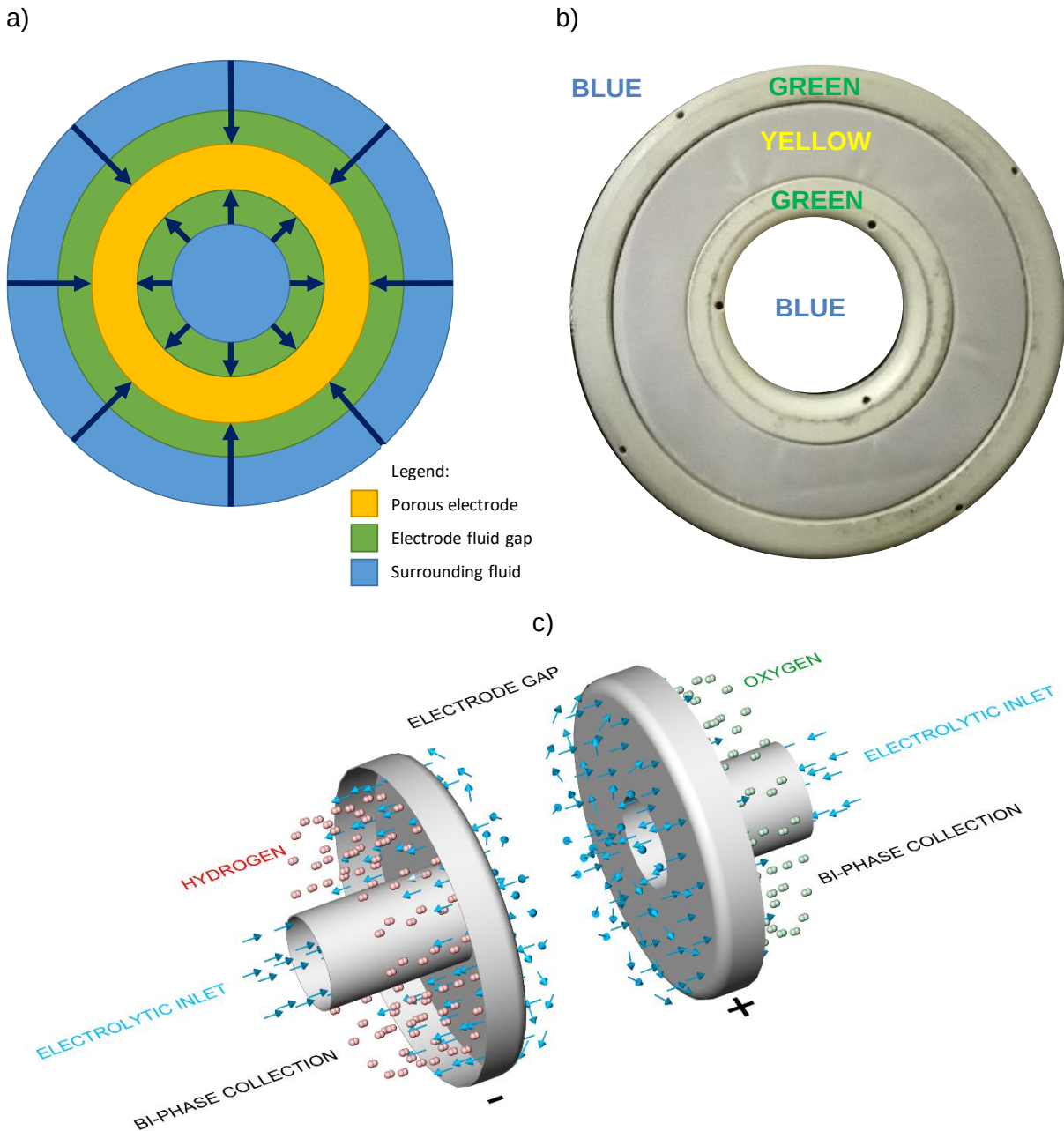


**Figure 3-2: Flow mechanism for injection into an annulus electrode design a) schematic representation, b) depicting image, and rendering showing central electrolyte injection.**

By allowing fluid to flow from the inner and outer annulus, a design was created that does not limit the outer diameter of the electrode, along with maintaining all other optimally deduced experimental parameters to remain in a designated range. Utilising two peripheral injections reduces the frontal gaseous meniscus in contrast to the prior MCFP approach. Previously, a parabolic pressure/velocity gradient was present across the circular electrode surface, as noted in Section 1.2.1.1. The pressure/velocity is greatest at the point of injection (circumference) and reduces across the face of the electrode, which implies that the flux across the electrode is not

uniform. Gas would, hence, find the path of least resistance at the central frontal region of the electrode due to insufficient solution flow present to drive gas through the porous electrodes. The new operating flow principle, as described in Figure 3-2, alleviates this issue to a greater extent employing electrolytic injection from two peripherals. The flux across the electrode is consequently more uniform, allowing for a reduced gas meniscus thickness across the electrode flow path. This theory would drive a further reduction in the minimum required flow velocity to maintain separation of the produced product gases while allowing for greater flow paths. Challenges that required solutions to this approach were:

- supplying the electrode with elevated amperages to account for the enhanced electrode surface area,
- limitation of the electrode diameter as a function of supporting plate thickness, and
- a floating inner electrode support ring that required anchorage without impeding the flow of electrolyte.

### **3.2.1.2 Introduction of a Non-conductive Mesh**

A novel method of dictating bubble formation on a porous electrode was employed by adhering a non-conductive mesh with specific well-defined uniform micron ratings onto the electrode surface. The idea intends to prevent/hamper the formation of gas on the frontal electrode surface. The non-conductive mesh, much like the electrode mesh, easily allows for gas and ions to move through its structure, and hence is effective at allowing the free-flow of electrolyte and consequently the free flow of ions. With a typical particle classification of 5  $\mu\text{m}$  to 1 mm at 1 A.cm<sup>-2</sup>, the non-conductive mesh would assist in preventing large bubble sizes (with the greatest buoyancy forces) from entering the electrode gap, however, smaller bubble sizes would be able to pass through this mesh structure [102]. Through the addition of a low diverging flow through this surface and the porous electrode, gas bubbles would successfully be prevented from entering the electrode gap. Consequently, movement of gas bubbles will be encouraged to the interstitial and rear region of the electrode. Low diverting flow can be achieved at higher velocities due to the velocity enhancement that is provided by the aperture restrictions of the non-conductive mesh. In addition, the flux distribution across the surface of the electrodes can be controlled by changing the aperture of the non-conductive mesh.

The face-to-face visible area reduction between the cathode and anode and the reduction in the rate of bubble removal from the surface of the electrodes, associated with the reduced flow rates, ultimately works to increase cell resistances and reduce current densities, however, a large gain in terms of the reduced parasitic loads was anticipated with a possible 20-75 times reduction in

flow in comparison to the prior deemed optimal flow velocity of  $0.075 \text{ m.s}^{-1}$ . This is significant in improving the overall efficiency of the plant and allowing for operation at significantly lower cell potentials. Previously operating at elevated cell voltages (low stack efficiencies) at the flow velocity of  $0.075 \text{ m.s}^{-1}$  would prove to yield the best overall efficiency conditions, however, the introduction of the non-conductive mesh would have the desired effect of reducing the operating cell voltage, as high current densities would no longer be needed to offset high parasitic loads.

### 3.2.2 Bi-MCFP Prototype Design

The incorporation of the annulus electrode design, with the requirement of having internal and external circumferential flow culminated into the design of a prototype termed Bi-MCFP (Bi-circumferential multiple circular filter press). A flow path of 20 mm was selected as a slight improvement over the 15 mm maximum to investigate the stipulated design modifications to the MCFP stack while still staying in the realm of what has been previously achieved. A reasonable electrode size was selected to accommodate a mono-polar design while still being mindful of the costs associated with the required internal busbar connections. The sizing of the electrode internal diameter was selected to account for a minimum required pipe diameter of the central inlet manifold, which was specified to be large enough to feed all electrodes with sufficient flow. Figure 3-3 provides a schematic of the electrode configuration as well as an image of the MCFP vs Bi-MCFP electrode structure, which has the following specifications:

- Outer diameter ( $D_{oe}$ ): 110 mm
- Inner diameter ( $D_{ie}$ ): 70 mm
- Electrode width: 40 mm
- Resulting flow path: 20 mm
- Intra electrode electrolytic feed tube diameter ( $D_{intra-flow}$ ): 50 mm
- Electrode fluid injection path length ( $L_{fp}$ ): 10 mm
- Electrode gap width ( $L_{eg}$ ): 20 mm
- Electrode Area:  $56.5 \text{ cm}^2$

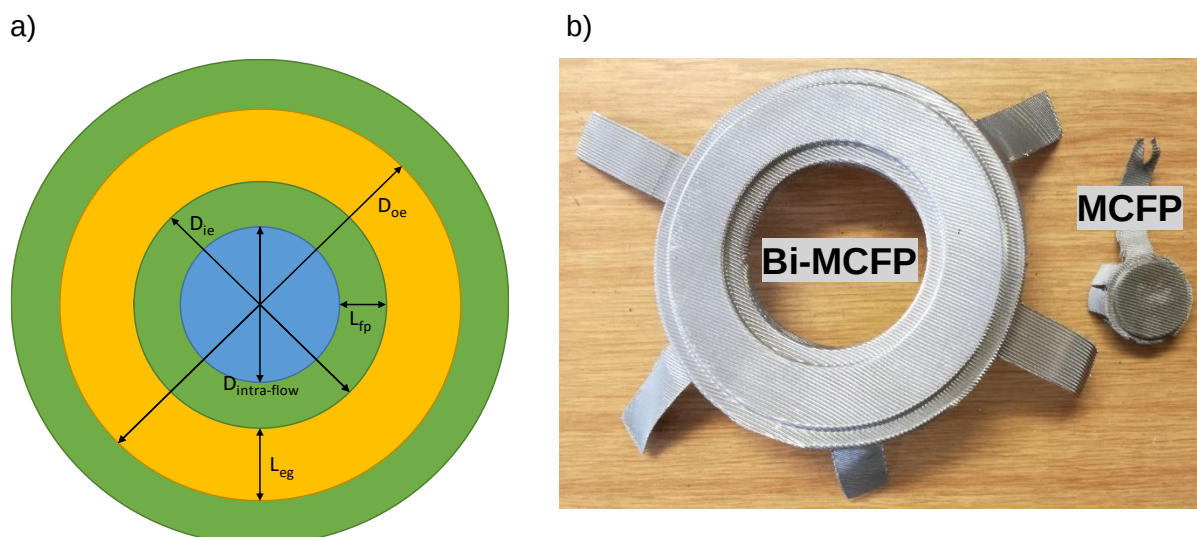


**Figure 3-3: Representative schematic of a) the Bi-MCFP electrode design and imagery showing the size comparison between b) the Bi-MCFP electrode to the MCFP electrode**

A Bi-MCFP reactor prototype was designed to house this electrode structure. To limit the amount of turbulence experienced within the reactor and electrode gap, all injection zones, for the electrode gap, make use of filleted reducing flow paths of radius 5 mm, the same radius currently employed by the working MCFP reactor prototype. The cross-sectional electrode area was calculated to be  $56.55 \text{ cm}^2$ . This represents an eight-fold increase in electrode area per cell when compared to the prior MCFP design. A schematic of the Bi-MCFP reactor prototype is provided in Figure 3-4.

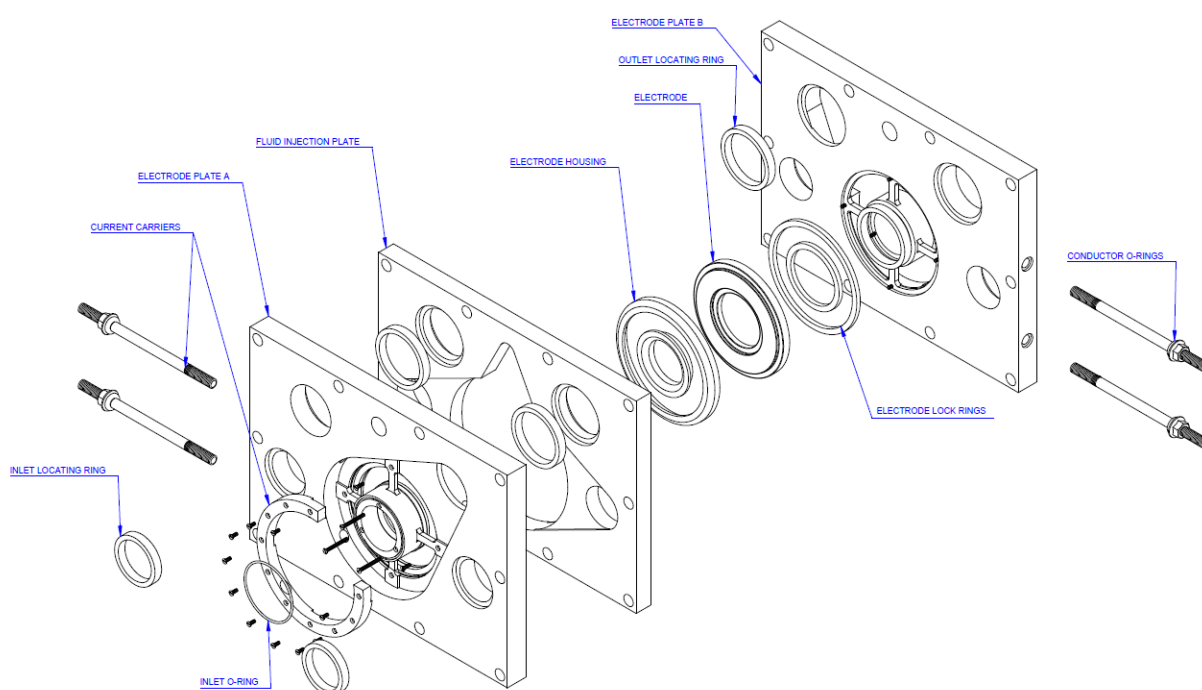


**Figure 3-4: Exploded view of the Bi-MCFP electrolyser prototype**

A Bi-MCFP cell makes use of a cathodic, anodic, and injection plate. The injection plate is recessed on the sides to permit flow from the internal injection manifolds to the injection chamber where it is then injected circumferentially to an electrode pair. A central injection manifold is created in the inner annulus of each electrode through a series of threaded connections. A purge chamber is incorporated in the injection plate would allow for gas that enters the electrode gap to be purged from the cell. Nickel current carriers (busbars) are provided to carry power in a unipolar connection (parallel connection) to the individual electrodes. The current carriers work based on a lock pin design, as shown in Figure 3-5. These were then inserted from the sides of the cell, which were locked in place to seal with an o-ring.

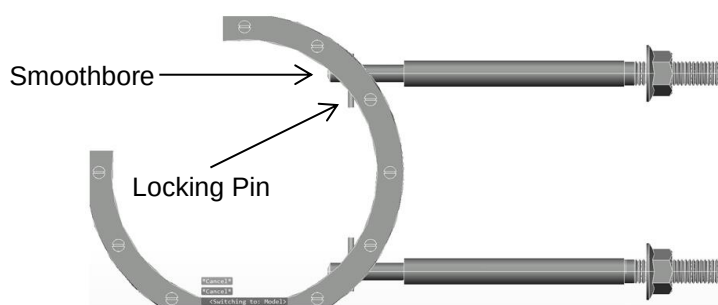


**Figure 3-5: Bi-MCFP current carrier**

The cells are then locked in place with locking rings inserted into the manifold chambers to later compress in a filter press design to form a larger multi-cell stack. A conceptualised assembly of a typical Bi-MCFP stack is illustrated in Figure 3-6.

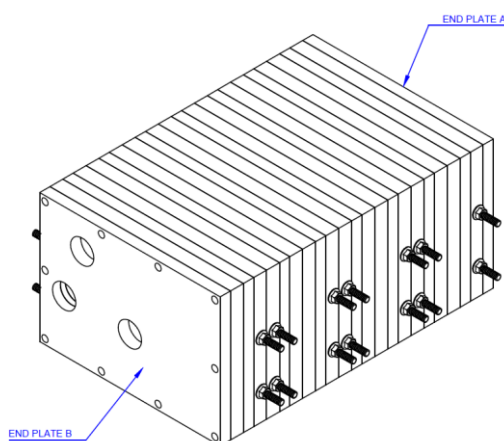


**Figure 3-6: Assembled view of a bi-circumferential reactor prototype stack**

Considering the reactor footprint of the prior MCFP design and contrasting that to the new Bi-MCFP approach, the following table, Table 3-1, provides a comparison of deduced production rates (assuming operation at  $1 \text{ A.cm}^{-2}$ ) as a function of single-cell volume.

**Table 3-1: Bi-MCFP and MCFP reactor production comparison from a single cell operating at 1 A.cm<sup>-2</sup>**

| Comparison Parameter                                        | Unit of Measurement                   | MCFP reactor pair | Bi- MCFP reactor pair |
|-------------------------------------------------------------|---------------------------------------|-------------------|-----------------------|
| Area of electrode                                           | cm <sup>-2</sup>                      | 7.07              | 56.55                 |
| Total amperage at 1 A.cm <sup>-2</sup>                      | A                                     | 7.07              | 56.55                 |
| Cell volume                                                 | cm <sup>3</sup>                       | 1 155             | 6 555                 |
| Mass production rate                                        | kg/day H <sub>2</sub>                 | 0.0064            | 0,051                 |
| Volumetric production rate                                  | NL/day H <sub>2</sub>                 | 77.15             | 617.20                |
| Mass production fn. stack volume                            | Kg/m <sup>3</sup> .day H <sub>2</sub> | 5.54              | 7.78                  |
| Volumetric production fn. Stack volume                      | NL/m <sup>3</sup> .day H <sub>2</sub> | 66971             | 94050                 |
| Hydrogen production fn. Stack volume percentage improvement | %                                     |                   | 40.4%                 |

### 3.2.3 Bi-MCFP Test Rig

#### 3.2.3.1 Balance of Plant

A test rig was developed to test multiple Bi-MCFP reactor configurations coupled to two gas/liquid separation options. The rig, consequently, comprised of many temporary components (mainly surrounding the system's piping) that could easily be interchanged. The rig by no means represents the finalised configuration for the 3 - 5 kg/day H<sub>2</sub> system, however, it contains the basic system components to obtain gas purity and performance data. Flow can be fed to the electrode gap from the inner manifold only, or by both the inner and outer manifolds. The central manifold has electrolytic solution introduced from both endplates, while the outer manifolds make use of solution injected from one end plate only, in a counter-current fashion, to balance the flow of electrolyte to all electrode pairs. The prototype stack comprised of a maximum of four electrode pairs, with the endplates. Some injection plates were fabricated from a translucent material to note the inner workings of the reactor.

As calculated previously, each electrode pair has a total cross-sectional cathodic area of 56.6 cm<sup>2</sup>, and hence the prototype stack had a total cathodic electrode area of 226.2 cm<sup>2</sup>. The test rig contained the following components:

1. 2.2 kW mag-drive pump
2. Electronic flowmeter
3. Electrolyte Filter
4. Bi-MCFP 4 Cell reactor
5. 3 kW heating Element
6. Pt100 temperature transmitter
7. Electrochemical gas analyser
8. Gas bubblers/flashback arrestor
9. Purge chamber float valve
10. Control and power conditioning cabinet
11. O<sub>2</sub> and H<sub>2</sub> gas lye separators
12. Level sensors on lye separators
13. Condensate traps
14. Demineralised water dosing pump

In addition to the items listed above hollow fibre membrane contactors with connected vacuum pumps were installed into the test rig. The hollow fibre membrane contactor was investigated as a means of gas-lye separation. The results of which will not be presented in this study. Images of the test rig have been provided in Figure 3-7. The Bi-MCFP test rig is similar in construction to that of the MCFP test rig that was communicated earlier [22].

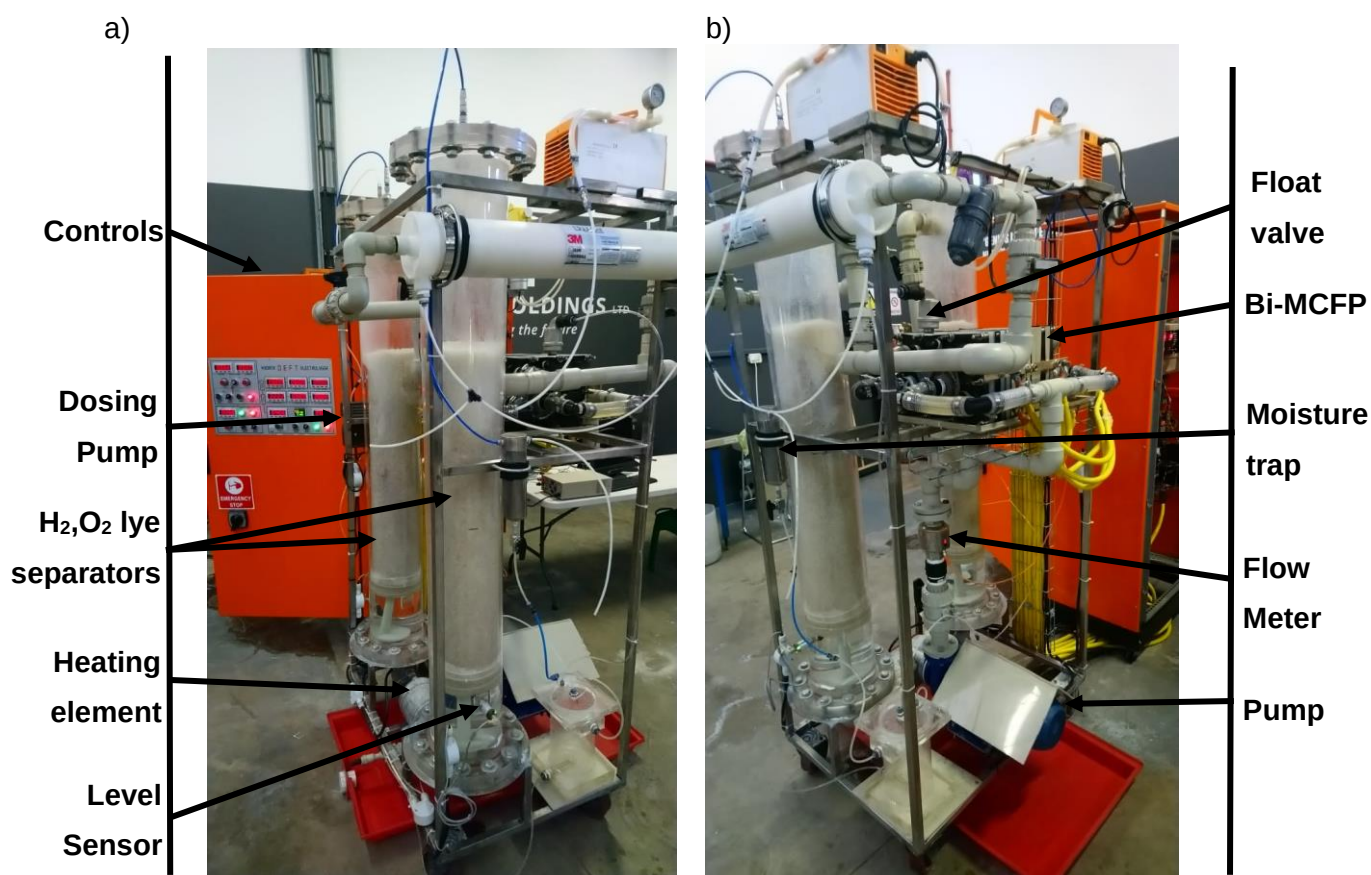


**Figure 3-7: a) Front view, and b) rear view images of the Bi-MCFP test plant.**

Hydrogen and oxygen gases are generated in the Bi-MCFP reactor. A bi-phase stream comprising of gas (either oxygen or hydrogen) and electrolyte (30% potassium hydroxide) is produced from the electrolyser stack. These streams then report to a gas/liquid separation system to liberate the gas from the electrolytic solution. Upon liberation of the gas, the electrolytic solution

is re-circulated employing a mag-drive centrifugal pump back into the reactor system. The produced hydrogen and oxygen gases are bubbled through a head of demineralised water to remove any residual KOH and, additionally, to act as a rudimentary flashback arrestor, from which the purity of the gas is measured by the provided electrochemical cell.

The test plant was generally operated at  $<80^{\circ}\text{C}$ , as the plant struggled to meet this temperature due to high heat losses being quite noticeable through the plant's components. Secondly, the systems handling of the removal of condensate (moisture traps) was very basic making use of a simple absorbent cartridge. At higher temperatures, the cartridges rapidly became saturated with water thus affecting the pressure drop across the unit and consequently disturbing the level balance between the hydrogen and oxygen gas-lye separators. Data at  $80^{\circ}\text{C}$  was subsequently obtained, presented in Section 3.3.3, by throttling the system's pump to provide an additional source of heat.

### **3.2.3.2 Parameter Control and Recording**

Gas purity was monitored for both the hydrogen and oxygen streams employing an electrochemical cell with an accuracy of 3% of the full scale. Though the accuracy range is broad, the meter proved adequate in defining experimental conditions producing favourable gas purity results. For subsequent detailed sample analysis, an independent lab (AirSep Labs) was commissioned for the volumetric analysis of the constituent gases by utilising an Agilent 6890 gas chromatograph.

The chemical circulation pump was linked to an Emerson 2.2 KW VFD (variable frequency drive), that provided the function of providing fluid flow control at the selected flow velocity. The PLC and test panel provided the added convenience of inputting and logging of process variables such as gas/liquid temperatures, solution flow rate, gas/liquid pressures along with stack amperages and voltages. Temperature was controlled at the desired set point utilising a PID controller. Stack amperages were generated through a variable switch mode power supply capable of providing 1200 amperes at a maximum cell potential of 10 VDC. The switch-mode power supply draws three-phase, 380 VAC, and had a turndown ratio of 10%, an electrical efficiency of 86% and a power factor of 92%. A Siemens S7 1200 PLC making use of TIA SCADA software was utilised to record and control some process variables. Various safety interlocks were built into the PLC software along with analogue safety interlocks to allow the plant to operate for extended time durations.

To provide control, or baseline, for the anodic and cathodic overpotential throughout over the

period of study, and for focusing on the optimisation of the reactor configuration, nickel 200 electrodes formed the basis of all investigations. The electrodes consisted of 80  $\mu\text{m}$  Ni 200 plain dutch weave woven mesh, supplied by Anping County Bolin Metal Wire Mesh Co., Ltd., Hebei Province, China. The surface of each electrode was etched in 17% HCl solution, supplied by Minema Chemicals (Pty) Ltd, Johannesburg, South Africa, for 4 minutes at an anodic current density of  $500 \text{ mA.cm}^{-2}$ . This yielded a chemically roughened surface suitable for gas nucleation due to the presence of multiple irregularities.

Type II distilled water, supplied by Labchem (Pty) Ltd, Johannesburg, South Africa, with a maximum specific conductance of  $0.05 \text{ uS.cm}^{-1}$  (ASTM, D1193-91) was used for all experimental investigations, with the solute being potassium hydroxide flakes of  $>90\%$  KOH, supplied by Kayo Fine Chemicals cc, Germiston, South Africa, with the balance being inert chemicals and sodium hydroxide.

The following major design attributes were investigated experimentally:

1. The reactor makes use of circumferential flow along the periphery of the electrode upon entering the electrode gap, both for the inner and outer radius. An image of the stack, as well as the liquid flow connections, is provided in Figure 3-8. The outer radius injection is, however, optional and consequently, two configurations were assessed:
  - inner and outer radius periphery injection, and
  - inner radius periphery injection.
2. Introduction of a non-conductive mesh on the frontal surface of the electrode to minimise gas formation within the electrode gap to aid in the reduction of plant-parasitic loads contributed by the pump,
  - as a function of flow rate (including ultra-low flow tests), and
  - as a function of micron rating.
3. Single-layer mesh type performance analysis.
4. Double-layer mesh type performance analysis.
5. Independent laboratory purity analysis of gas formed by the reactor.
6. Durability analysis of the reactor.

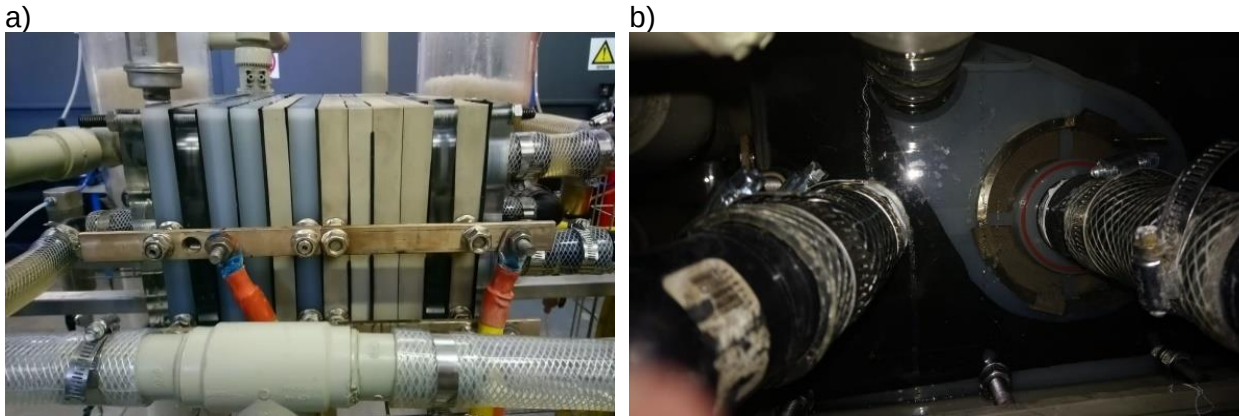


**Figure 3-8: a) Bi-MCFP electrolyser stack, and b) Liquid electrolyte manifold connections**

To provide conciseness to the report, not all results are provided for the sections to follow, only those that would provide a clear conclusion to the particular sub-section. With the conclusion of the above tests, a finalised configuration of the reactor was outlined to move forward into large scale demonstration work.

For each of the set experimental conditions, experiments were repeated 3 times to gain a sense of the repeatability of experimental results. Experimental analysis of results was performed by calculating the standard deviation and uncertainty for each data set.

### **3.3 Results and Discussion**

#### **3.3.1 Electrolyte Injection Configuration**

Electrolyte inlet configuration comparisons were conducted before the non-conductive mesh was integrated into the Bi-MCFP stack, with results presented in Figure 3-9. This was done in the effort to obtain a benchmark for determining performance losses/gains associated with further design modifications. In this case, the Bi-MDFP reactor was operated at flow velocities comparable to the operation of the MCFP stack that was reported earlier [1], [22]. It is expected that the use of injection from both the inner and outer radii should have the most favourable effect as flow distribution would be most uniform. The flow path effectively would be substantially shorter, however, the incorporation of three electrolyte injection manifolds adds complexity and cost to the design.

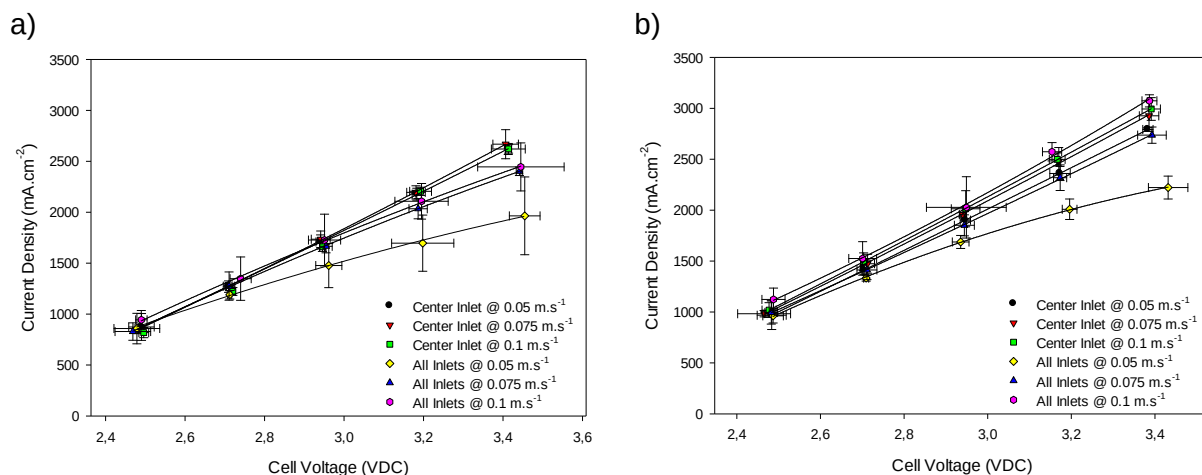


**Figure 3-9: Polarisation curves for (a) 50°C and (b) 60°C for the Bi-MCFP stack utilising no non-conductive mesh at an electrode gap of 2.5 mm, utilising 80  $\mu\text{m}$  PD weave, 30% KOH as a function of flow velocity**

At 50°C it was noted that the central inlet only configuration appears to maximise performance for all flow velocities (Figure 3-9a). The curves additionally show very little variance with flow velocity. Figure 3-9b, at a higher temperature of 60°C, noted the trend of highest current density results for the configuration employing all electrolytic inlets operating at a flow velocity of 0.1  $\text{m.s}^{-1}$ , however, this curve is closely followed by results for the central (inlet flow velocity of 0.1  $\text{m.s}^{-1}$ ). The annulus design configuration notes similar current densities to that reported in literature for the MCFP reactor prototype [22]. Table 3-2 provides polarisation data comparisons between the Bi-MCFP and MCFP reactor at 60°C and 0.075  $\text{m.s}^{-1}$ .

**Table 3-2: Polarisation data for the Bi-MCFP and MCFP reactor at 60°C, flow velocity 0.075  $\text{m.s}^{-1}$  of flow velocity, 80  $\mu\text{m}$  PD weave Nickel electrodes**

| Bi-MCFP All inlets |                                         | Bi-MCFP Central inlets |                                         | MCFP [1], [22] |                                         |
|--------------------|-----------------------------------------|------------------------|-----------------------------------------|----------------|-----------------------------------------|
| Voltage (VDC)      | Current Density ( $\text{mA.cm}^{-2}$ ) | Voltage (VDC)          | Current Density ( $\text{mA.cm}^{-2}$ ) | Voltage (VDC)  | Current Density ( $\text{mA.cm}^{-2}$ ) |
| $2.48 \pm 0.015$   | $1000.9 \pm 114.5$                      | $2.46 \pm 0.063$       | $988.8 \pm 31$                          | 2.5            | 999.3                                   |
| $2.94 \pm 0.024$   | $1856.5 \pm 103.3$                      | $2.94 \pm 0.008$       | $1962 \pm 23.5$                         | 3              | 1740.1                                  |
| $3.39 \pm 0.034$   | $2741.9 \pm 80.2$                       | $3.39 \pm 0.023$       | $2931.7 \pm 152.5$                      | 3.5            | 2883.4                                  |

### 3.3.2 Non-Conductive Mesh Micron Ratings

The mesh is comprised of well-defined apertures and is manufactured from a polyamide polymer (Nylon). Materials selection for the mesh, however, could be improved. Nylon, however, was selected due to its widespread availability in a broad range of micron ratings and due to its relatively high resistance to short-term chemical attack. Three different micron ratings, 5  $\mu\text{m}$ , 10  $\mu\text{m}$ , and 25  $\mu\text{m}$ , were analysed during this investigation to note their effect on cell performance. The non-conductive mesh was installed into the cell by stretching it over the surface of the electrode and locking it in place under the same mechanism as that of the nickel electrode. Figure 3-10 provides images of the non-conductive mesh installed into a cell.

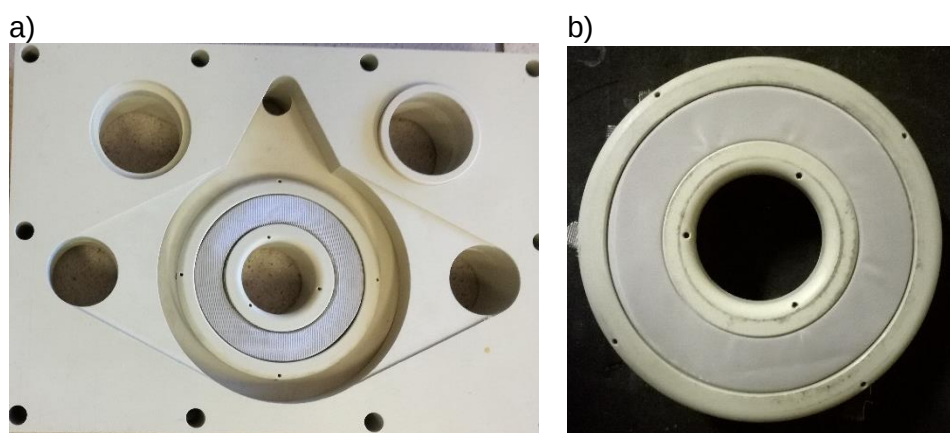


**Figure 3-10: Installation of the non-conductive mesh into the Bi-MCFP cell**

For flow velocity selection, the 25  $\mu\text{m}$  non-conductive mesh was installed into the cell. The flow rate, and hence flow velocity, was adjusted until some purge gas evolution (gas entering the electrode gap) was noted. A flow rate above this point was then selected as the demonstrative flow rate/flow velocity. This value was determined to be 0.004  $\text{m.s}^{-1}$ , which culminates into a 18.75 times reduction in flow from the original 0.075  $\text{m.s}^{-1}$  MCFP operating point. Figure 3-11 provides IV data for the operation with non-conductive mesh aperture ratings of 5  $\mu\text{m}$ , 10  $\mu\text{m}$ , and 25  $\mu\text{m}$ .

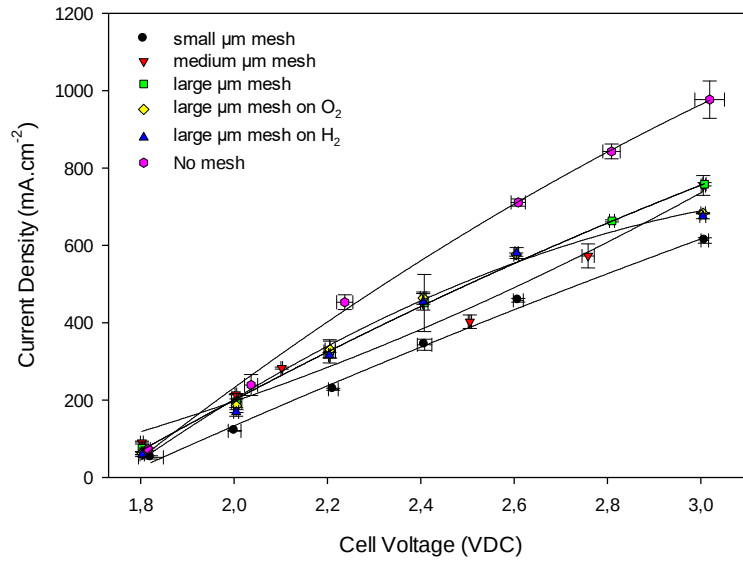


**Figure 3-11: Polarisation curves for the Bi-MCFP stack utilising a variation of non-conductive mesh aperture ratings at an electrode gap of 2.5 mm, utilising 80 µm DW weave, 30% KOH, 60°C, at a flow velocity of 0.004 m.s<sup>-1</sup>**

The results are coherent with the expectation that current density would reduce with reducing aperture sizes. The Bi-MCFP stack was operated with no non-conductive mesh at 0.004 m.s<sup>-1</sup> in order to assess what performance loss is associated with the flowrate reduction and what percentage loss is associated with the installation of the non-conductive mesh. An experiment was carried out by adding the mesh only to one electrode, being either the anode or the cathode. The performance was similar to the mesh being present on both electrodes, which implies that the thickness has little influence on the performance, and instead the porosity has the presiding significance, similar to the normal operation of porous electrodes. It is further noted that the gradient of the IV curve for operation without a non-conductive mesh is not constant with a drop off in slope at higher voltages. This is as a result of the reduced effect of bubble removal from the cell at the lower flow velocities, hence, the high void fraction at high current densities increases the cell resistance as a consequence. Table 3-3 provides the change in current density with the reduction of flow velocities and the introduction of a non-conductive (NC) mesh.

**Table 3-3: Change in IV characteristics with the implementation of design modifications (flow rate with/without NC mesh).**

| High Flow no NC Mesh |                                         | Low Flow no NC Mesh |                                         | 25 $\mu\text{m}$ NC Mesh |                                         | 10 $\mu\text{m}$ NC Mesh |                                         | 5 $\mu\text{m}$ NC Mesh |                                         |
|----------------------|-----------------------------------------|---------------------|-----------------------------------------|--------------------------|-----------------------------------------|--------------------------|-----------------------------------------|-------------------------|-----------------------------------------|
| Voltage (VDC)        | Current Density ( $\text{mA.cm}^{-2}$ ) | Voltage (VDC)       | Current Density ( $\text{mA.cm}^{-2}$ ) | Voltage (VDC)            | Current Density ( $\text{mA.cm}^{-2}$ ) | Voltage (VDC)            | Current Density ( $\text{mA.cm}^{-2}$ ) | Voltage (VDC)           | Current Density ( $\text{mA.cm}^{-2}$ ) |
| -                    | -                                       | $1.8 \pm 0.01$      | $75 \pm 3.1$                            | $1.8 \pm 0.01$           | $77 \pm 6.4$<br>(-3%)                   | $1.8 \pm 0.01$           | $92 \pm 5.7$<br>(-23%)                  | $1.8 \pm 0.03$          | $54 \pm 4.1$<br>(28%)                   |
| -                    | -                                       | $2.0 \pm 0.01$      | $241 \pm 27$                            | $2.0 \pm 0.01$           | $198 \pm 21$<br>(18%)                   | $2.0 \pm 0.01$           | $216 \pm 8.4$<br>(10%)                  | $2.0 \pm 0.01$          | $122 \pm 8.0$<br>(49%)                  |
| -                    | -                                       | $2.2 \pm 0.02$      | $454 \pm 19$                            | $2.2 \pm 0.01$           | $328 \pm 30$<br>(28%)                   | $2.2 \pm 0.02$           | $307 \pm 11$<br>(32%)                   | $2.2 \pm 0.01$          | $230 \pm 2.7$<br>(49%)                  |
| $2.4 \pm 0.03$       | $805 \pm 31$                            | $2.4 \pm 0.02$      | $535 \pm 12$<br>(34%)                   | $2.4 \pm 0.01$           | $453 \pm 73$<br>(15%)                   | $2.4 \pm 0.01$           | $410 \pm 4.3$<br>(23%)                  | $2.4 \pm 0.02$          | $345 \pm 14$<br>(36%)                   |
| $2.6 \pm 0.02$       | $1210 \pm 93$                           | $2.6 \pm 0.02$      | $713 \pm 9.3$<br>(41%)                  | $2.6 \pm 0.01$           | $543$<br>(24%)                          | $2.6 \pm 0.01$           | $512 \pm 6.4$<br>(28%)                  | $2.6 \pm 0.01$          | $460 \pm 4.7$<br>(35%)                  |
| $2.8 \pm 0.01$       | $1615 \pm 84$                           | $2.8 \pm 0.02$      | $845 \pm 19$<br>(48%)                   | $2.8 \pm 0.01$           | $665 \pm 12$<br>(21%)                   | $2.8 \pm 0.01$           | $575 \pm 8.9$<br>(32%)                  | $2.8 \pm 0.01$          | $529 \pm 9.3$<br>(37%)                  |
| $3.0 \pm 0.02$       | $2020 \pm 92$                           | $3.0 \pm 0.03$      | $979 \pm 48$<br>(52%)                   | $3.0 \pm 0.01$           | $760 \pm 14$<br>(22%)                   | $3.0 \pm 0.01$           | $757 \pm 11$<br>(23%)                   | $3.0 \pm 0.01$          | $615 \pm 7.1$<br>(37%)                  |

\*Percentage decrease from high flow ( $0.075 \text{ m.s}^{-1}$ ) no NC mesh.

\*Percentage decrease from low flow ( $0.075 \text{ m.s}^{-1}$ ) no NC Mesh.

Trying to maximize the current density at a set voltage is a priority, however, ultimately the determining factor governing which non-conductive micron rate may be successfully implemented is the extent of gas separation i.e. the gas purity. For this assessment, a basic analysis of gas purity was performed using an electrochemical cell with an accuracy of 3% of the full scale. Non-conductive mesh aperture rating variations and configurations were tested over an array of current densities operating at  $0.004 \text{ m.s}^{-1}$ . Steady-state hydrogen gas purities were monitored during operation. Figure 3-12 provides the results of this study.

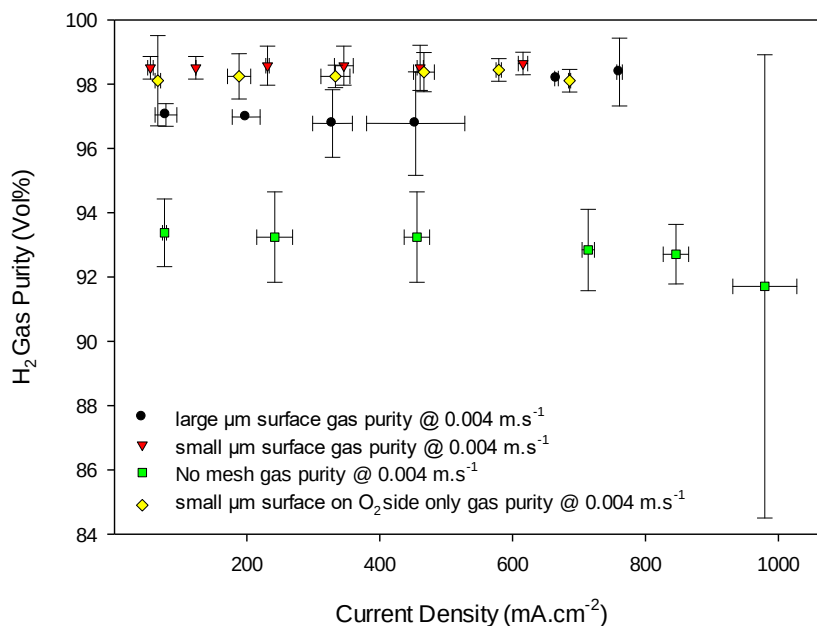


**Figure 3-12: Gas purity versus current density for a variation of mesh micron ratings at a temperature of 60°C, 80 μm dutch weave, electrode gap of 2.5 mm, 30% KOH and a flow velocity of 0.004 m.s<sup>-1</sup>**

Gas purities were considered as a function of a few of the surface configurations tested. It is noted that the larger 25 μm rating did not produce adequate gas purities with values approaching the 97 vol% H<sub>2</sub> mark. Although this is higher than the H<sub>2</sub> in O<sub>2</sub> high explosive limit (HEL) it is lower than the industrial benchmark of >99 vol% H<sub>2</sub>, which is considered a satisfactory safe operating limit. Poor gas purities were noted (below the HEL) for operations without a non-conductive layer at 0.004 m.s<sup>-1</sup>. Although this was expected it additionally stresses the importance that when operating DEFT™ at low flow velocities, it must be performed in combination with the non-conductive mesh. The low 5 μm mesh was capable of maintaining gas purities of >99 vol% H<sub>2</sub> over the current density range. It was, however, believed that the actual gas purity produced by the stack was higher as the plant was found not to be entirely air-tight with some leaks found in gas pipeline fittings. It was also noted that the gas lye separators were not operating at 100% separation efficiency, therefore, some entrapped gas may have been recycled.

To ascertain a more representative measure of gas purities produced by the stack, the bi-phase solutions were directed from the outlet of the stack to the membrane contractors. Hollow fibre membrane contactors are commonly utilised in industry to remove dissolved gas from processing streams. This allowed for a controlled gas purity measurement without the error provided by imperfect separation efficiencies and gas leaks. In this case, 4 samples (2 hydrogen stream and 2 oxygen stream samples) were collected by an independent gas analysis company (as noted in Section 3.2.3.2) for GC measurement. The process conditions were selected at 500 mA.cm<sup>-2</sup>,

60°C, 5  $\mu\text{m}$  non-conductive mesh and a further reduced flow velocity of 0.001  $\text{m.s}^{-1}$ . This flow velocity represented the lower limit of the test plant's pumping system. The results of the independent laboratory analysis can be found in Appendix B, following the embodiment of this report. An extract from the report is provided in Table 3-4.

**Table 3-4: Gas purity results for a 5  $\mu\text{m}$  non-conductive mesh operating at 500  $\text{mA.cm}^{-2}$ , 60°C and 0.001  $\text{m.s}^{-1}$ .**

**CERTIFICATE OF ANALYSIS 18-280**

**ANALYSIS OF GAS SAMPLES**

| Sample | Test Result (%) |                |                | Uncertainty of result |
|--------|-----------------|----------------|----------------|-----------------------|
|        | H <sub>2</sub>  | O <sub>2</sub> | N <sub>2</sub> |                       |
| "S1"   | 99.81           | 0.05           | 0.14           | $\pm 0.1 \%$          |
| "S2"   | 99.70           | 0.10           | 0.20           | $\pm 0.1 \%$          |
| "S1"   | < 0.2           | 99.35          | 0.45           | $\pm 0.1 \%$          |
| "S2"   | < 0.2           | 99.28          | 0.52           | $\pm 0.1 \%$          |

Gas purity samples were extracted from the Bi-MCFP test plant once it had been operating for more than 48 hours. With reference to the result, it is noted that 'S1' and 'S2' for the hydrogen separator measured gas purities above 99.5 vol%. Samples 'S1' and 'S2' for the oxygen separator are noted to be below the benchmark of 99.5 vol%, with the majority of the contaminate being nitrogen. This indicates the presence of atmospheric contaminants, which may have entered the sample during the gas sampling process. Discounting the nitrogen result would have developed an oxygen result greater than 99.5 vol%.

### 3.3.3 Effect of Flow Velocity on Performance

The trend concerning flow velocity is the same as for prior investigations. An increase in flow velocity reduces the residence time that bubbles spend on the surface of an electrode. It additionally has several other advantages, namely, reduction of concentration gradients, enhanced distribution of heat, improvement in mass transfer resistances and aiding in breaking down the double layer. Although these advantages are welcomed, DEFT™'s main utilisation of

flow is gas separation. A balance, however, must be struck between the load consumed by the pump for generating the flow, and the benefit gained from the flow in enhancing the performance of the reactor. In this section, this relationship will be investigated in detail, to assess whether the benefits provided by increased flow operation out-weigh the additional parasitic load requirement in the effort to reduce overall system power consumptions. To carry out this investigation IV data (provided in Figure 3-13) was generated for a 25  $\mu\text{m}$  non-conductive mesh at flows that extended down to the test plant's lower pumping limit. A 25  $\mu\text{m}$  non-conductive mesh was chosen to provide the study with a maximum current density point.

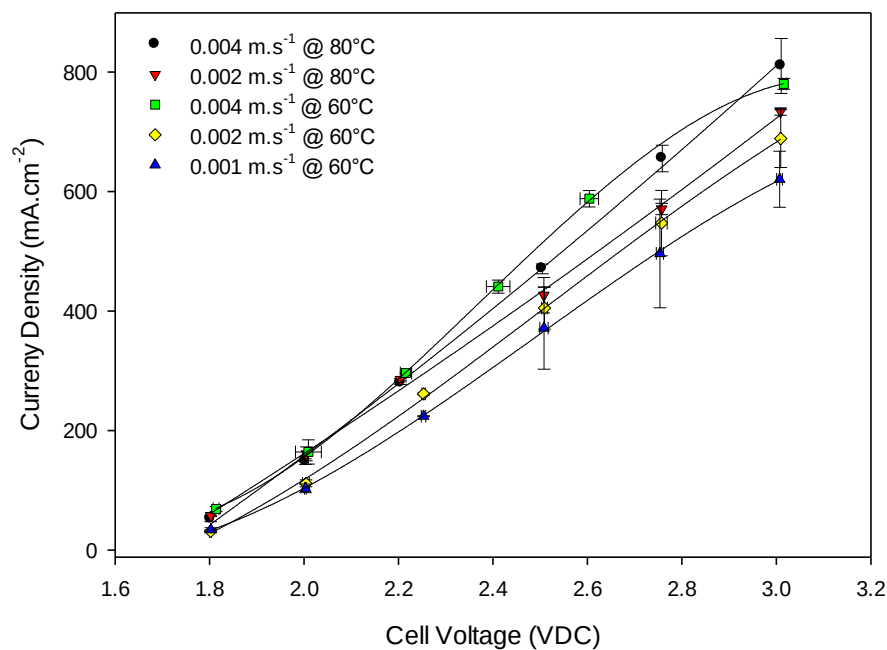


**Figure 3-13: Polarisation curve for the Bi-MCFP reactor for 80  $\mu\text{m}$  DW, 25  $\mu\text{m}$  non-conductive mesh, an electrode gap of 2.5 mm, 30% KOH and 60°C**

It is clear to note the enhancement of performance from 0.002  $\text{m.s}^{-1}$  to 0.004  $\text{m.s}^{-1}$ , at higher operating potentials (high current densities) which is greater in comparison to the increase from 0.001  $\text{m.s}^{-1}$  to 0.002  $\text{m.s}^{-1}$ . This is because at high current densities, increased void fraction from extensive bubble creation, increases cell resistances. Operating at the low flow velocities provides little additional benefit to the performance of the stack at low voltages where bubble resistance has a lesser effect. At 1.8 VDC the performance gain from 0.001  $\text{m.s}^{-1}$  to 0.002  $\text{m.s}^{-1}$  is negligible, however, the parasitic load of the pump doubled.

Table 3-5 shows the resulting flowrate as a consequence of operating at various electrolytic velocities.

**Table 3-5: Comparison of required solution flow rates with reducing flow velocities as a function of operating current density based on Ni dutch weave 80  $\mu\text{m}$  and a temperature of 60°C**

| Target<br>Production<br>Rate<br>(kg/day H <sub>2</sub> )                                 | Total<br>Amperage<br>Required<br>(A) | Cell<br>Potential<br>(VDC) | Current<br>Density<br>(mA.cm <sup>-2</sup> ) | Flow<br>Velocity<br>(m.s <sup>-1</sup> ) | Required<br>Electrode<br>Area of<br>cathode<br>(m <sup>2</sup> ) | Total<br>Solution<br>Flow<br>(L/min) |
|------------------------------------------------------------------------------------------|--------------------------------------|----------------------------|----------------------------------------------|------------------------------------------|------------------------------------------------------------------|--------------------------------------|
| No Non-conductive mesh DEFT™ operating at 0.075 m.s <sup>-1</sup> using Ni 80 μm DW mesh |                                      |                            |                                              |                                          |                                                                  |                                      |
| 5                                                                                        | 5539.35                              | 1.80 ± 0.01                | 113.2 ± 12                                   | 0.075                                    | 4.89                                                             | 44049                                |
|                                                                                          |                                      | 2.00 ± 0.01                | 267.6 ± 8.6                                  |                                          | 2.07                                                             | 18629                                |
|                                                                                          |                                      | 2.20 ± 0.01                | 484.0 ± 22                                   |                                          | 1.15                                                             | 10302                                |
|                                                                                          |                                      | 2.41 ± 0.01                | 741.0 ± 34                                   |                                          | 0.7                                                              | 6728                                 |
|                                                                                          |                                      | 2.60 ± 0.01                | 1012 ± 61                                    |                                          | 0.55                                                             | 4929                                 |
|                                                                                          |                                      | 2.81 ± 0.01                | 1320 ± 54                                    |                                          | 0.42                                                             | 3777                                 |
| Non-conductive mesh DEFT™ operating at 0.004 m.s <sup>-1</sup> using Ni 80 μm DW mesh    |                                      |                            |                                              |                                          |                                                                  |                                      |
| 5                                                                                        | 5539.35                              | 1.80 ± 0.01                | 76.92 ± 6.4                                  | 0.004                                    | 7.20                                                             | 3457                                 |
|                                                                                          |                                      | 2.00 ± 0.01                | 197.8 ± 21                                   |                                          | 2.80                                                             | 1345                                 |
|                                                                                          |                                      | 2.20 ± 0.01                | 327.7 ± 30                                   |                                          | 1.69                                                             | 811                                  |
|                                                                                          |                                      | 2.41 ± 0.01                | 453.0 ± 73                                   |                                          | 1.22                                                             | 587                                  |
|                                                                                          |                                      | 2.81 ± 0.01                | 664.9 ± 12                                   |                                          | 0.83                                                             | 400                                  |
|                                                                                          |                                      | 3.01 ± 0.01                | 759.8 ± 14                                   |                                          | 0.73                                                             | 350                                  |
| Non-conductive mesh DEFT™ operating at 0.002 m.s <sup>-1</sup> using Ni 80 μm DW mesh    |                                      |                            |                                              |                                          |                                                                  |                                      |
| 5                                                                                        | 5539.35                              | 1.80 ± 0.01                | 32.72 ± 2.3                                  | 0.002                                    | 16.93                                                            | 4063                                 |
|                                                                                          |                                      | 2.00 ± 0.01                | 113.0 ± 5.9                                  |                                          | 4.90                                                             | 1177                                 |
|                                                                                          |                                      | 2.25 ± 0.01                | 262.7 ± 17                                   |                                          | 2.11                                                             | 506                                  |
|                                                                                          |                                      | 2.51 ± 0.01                | 406.5 ± 36                                   |                                          | 1.36                                                             | 327                                  |
|                                                                                          |                                      | 2.76 ± 0.01                | 548.6 ± 54                                   |                                          | 1.01                                                             | 242                                  |
|                                                                                          |                                      | 3.01 ± 0.01                | 690.1 ± 48                                   |                                          | 0.80                                                             | 193                                  |
| Non-conductive mesh DEFT™ operating at 0.001 m.s <sup>-1</sup> using Ni 80 μm DW mesh    |                                      |                            |                                              |                                          |                                                                  |                                      |
| 5                                                                                        | 5539.35                              | 1.80 ± 0.01                | 35.52 ± 2.3                                  | 0.001                                    | 15.60                                                            | 1871                                 |
|                                                                                          |                                      | 2.00 ± 0.01                | 104.6 ± 5.9                                  |                                          | 5.29                                                             | 635                                  |
|                                                                                          |                                      | 2.25 ± 0.01                | 225.4 ± 9                                    |                                          | 2.46                                                             | 295                                  |
|                                                                                          |                                      | 2.51 ± 0.01                | 372.8 ± 28                                   |                                          | 1.49                                                             | 178                                  |
|                                                                                          |                                      | 2.75 ± 0.01                | 497.9 ± 45                                   |                                          | 1.11                                                             | 134                                  |
|                                                                                          |                                      | 3.01 ± 0.01                | 622.0 ± 46                                   |                                          | 0.89                                                             | 107                                  |

The flows required for the original optimal flow velocity of 0.075 m.s<sup>-1</sup> proves to be impractical for scale-up even at high operating potentials/high current densities. This flow would then need to be substantially reduced by linking separator-reactor modules in series, for example. Significant current density enhancements would then be necessary to bring the overall plant efficiency in line with what can be expected with small scale electrolyzers. Introduction of the non-conductive mesh has yielded significant reductions in the required flow rate, however, as with the flow velocity of 0.075 m.s<sup>-1</sup>, flows that are manageable by simplistic gas/liquid gravitational separation methods are only achieved at high operating potentials (low voltage efficiencies).

To investigate the effect of flow velocity on the overall system efficiency, system power consumptions were determined for DEFT™ operating at various temperatures and flow velocities. At each condition, the current density was recorded at varying operating voltages in the range of 1.8 to 3 VDC. The data was obtained with a configuration/setup that incorporated the following:

IV Data was generated utilising:

- a 4 Cell DEFT™ electrolysis stack
- 30% KOH as electrolyte
- Utilising 24 x 110 (80 µm) plain dutch weave Ni 200 mesh (no additional catalytic coating)
- Utilising a single central electrolyte inlet
- Utilising a 5 µm non-conductive mesh
- Amperages below 60 A were recorded with a pure DC bench-scale power supply, supplied by Wuhan Guanyou New Energy Technology Co., Ltd. (brand: TMO, output voltage: 0-60 VDC, output current: 0-150 A). Amperages above 60 A were recorded with a larger rectified 5 mV pulsed DC power supply, supplied by Power Dynamics Ltd, Johannesburg, South Africa (Output voltage: 0-10 VDC, output current: 135 – 1350 A).

The overall power consumption was generated under the following assumptions:

- All pump power consumption values determined with an assumed pump efficiency of 50%.
- Overall system power determinations were based on estimated pump power consumptions (Eq. 1-1) and stack power consumptions. Balance of plant and AC/DC power conversion efficiencies were ignored. Consequently, the values provided do not give a true representation of system power consumptions, but rather a means of assessing the effect of flow rates and voltage selection on the overall power consumption.
- A system head of 0.1 bar pressure drop per electrode pair.

The larger pulsed DC power supply may provide an amperage that would not be consistent with a pure DC power supply at the same voltage, however, since all tests were subjected to the same conditions the trends, and hence the operation of each setup, can be compared. The power consumption curves, at 60°C and 80°C for various electrolytic velocities and operating potentials, are provided in Figure 3-14.

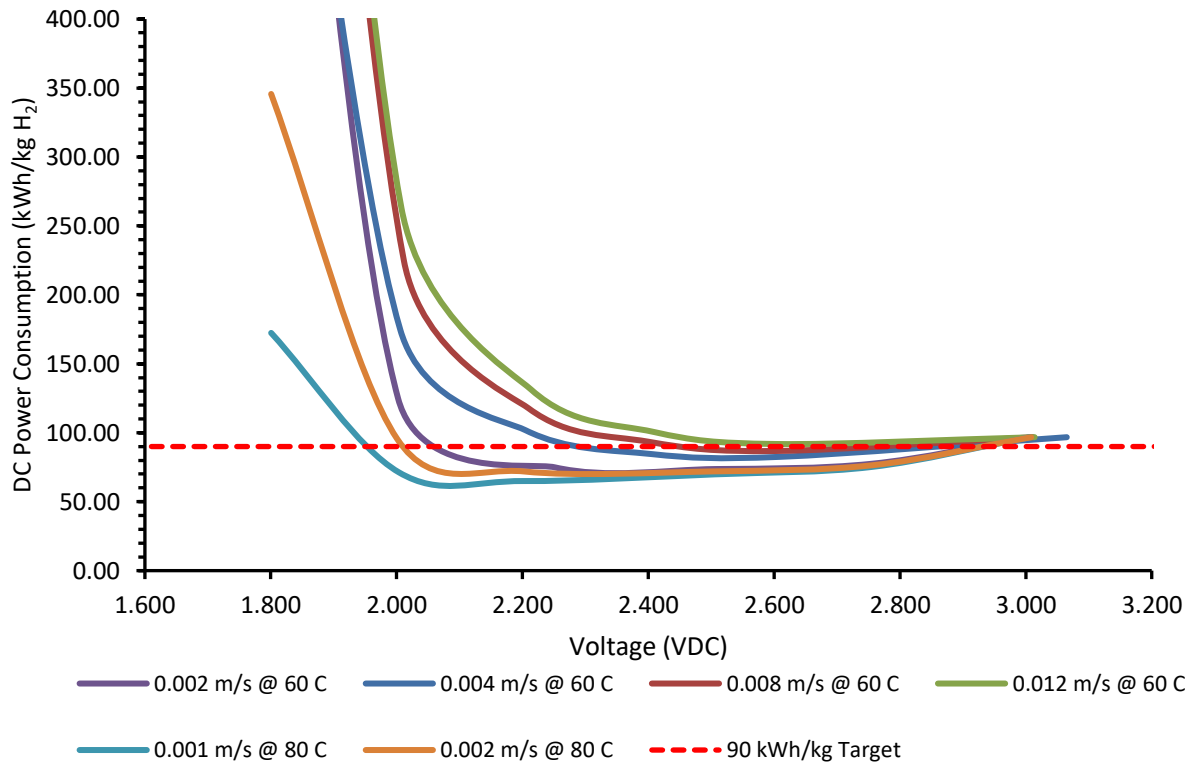


**Figure 3-14: Power consumption curves at 60°C & 80°C for variable electrolytic flow velocities and operating voltages**

The curves move further down the y-axis with decreasing flow rate and at no point do the curves intercept. This indicates that the overall efficiency increases with decreasing flowrate for all operating voltages within the selected range. It is apparent that the overall efficiency, under the conditions of the investigation, finds no overall benefit to the overall power consumption from the increased current density associated with increasing flowrates. This is because increasing the flowrate increases the pump power consumption by a greater factor than that seen for the increase in current density, therefore, increasing the electrolytic flow velocity always results in a decrease in the overall efficiency. For the increase in the electrolytic flow velocity to be beneficial towards the overall efficiency, the current density would need to increase by more than two-fold if the electrolytic flow velocity was doubled. In other words, the production rate (kg/hr H<sub>2</sub>) would need to increase as such to offset the larger power consumption (kWh) to realise a reduced overall efficiency (kWh/kg H<sub>2</sub>). Thus far the increase in current density, at low operating potentials, has been insignificant in comparison to the resultant increase in the pump power consumption due to the increase in the electrolytic volumetric flowrate. As current density gains through increased flow rates are not beneficial to the process' overall efficiency, the electrolytic flow velocity needs to be minimised to a point. It is noted that effective gas separation is achieved at the lowest volumetric flow-rate possible in order to minimise the overall power consumption.

The curves, representing the performance at higher flowrates, exhibit exponential decay in the overall power consumption at low voltages up until the inflection point at minimum power consumption. A low increasing gradient is then noted in power consumption with increasing voltage. This behaviour is a consequence of the fact that the volumetric flow rate required is based on an electrolytic flow velocity value ( $\text{m.s}^{-1}$ ), therefore, at low voltages and hence low current densities a large electrode area is required. Multiplying this by the velocity results in a large volumetric flow rate along with a larger pressure head requirement. Although the system is operating at a low voltage and low electrolytic flow velocity, the large volumetric flow rate as a consequence of the larger number of electrode pairs results in poor overall efficiencies. It is, however, noted that as the electrolytic flow velocity decreases the inflection point and hence the optimal/minimised overall power consumption shifts to the left of the x-axis towards lower voltages (higher voltage efficiencies).

Figure 3-14 shows that operations at  $80^{\circ}\text{C}$ , with electrolytic velocities of  $0.001 \text{ m.s}^{-1}$  and below, results in overall power consumptions below the  $90 \text{ kWh/kg H}_2$  target set out in Section 1.2.2 with a power consumption of  $65 \text{ kWh/kg H}_2$  ( $60.62 \text{ HHV}$ ) being achieved at  $2.2 \text{ VDC}$  with an electrode area of  $1.97 \text{ m}^2$ . Figure 3-15 provides an expanded view of the curve representing operation at  $80^{\circ}\text{C}$  at  $0.001 \text{ m.s}^{-1}$ . The figure depicts the portions that the pump and stack contribute towards the overall power consumption. Along with efficiency data, Figure 3-15 provides an estimation of the number of electrode pairs required, assuming an electrode with a  $350 \text{ cm}^2$  geometric area, to allow for a  $5 \text{ kg/day H}_2$  production capacity.

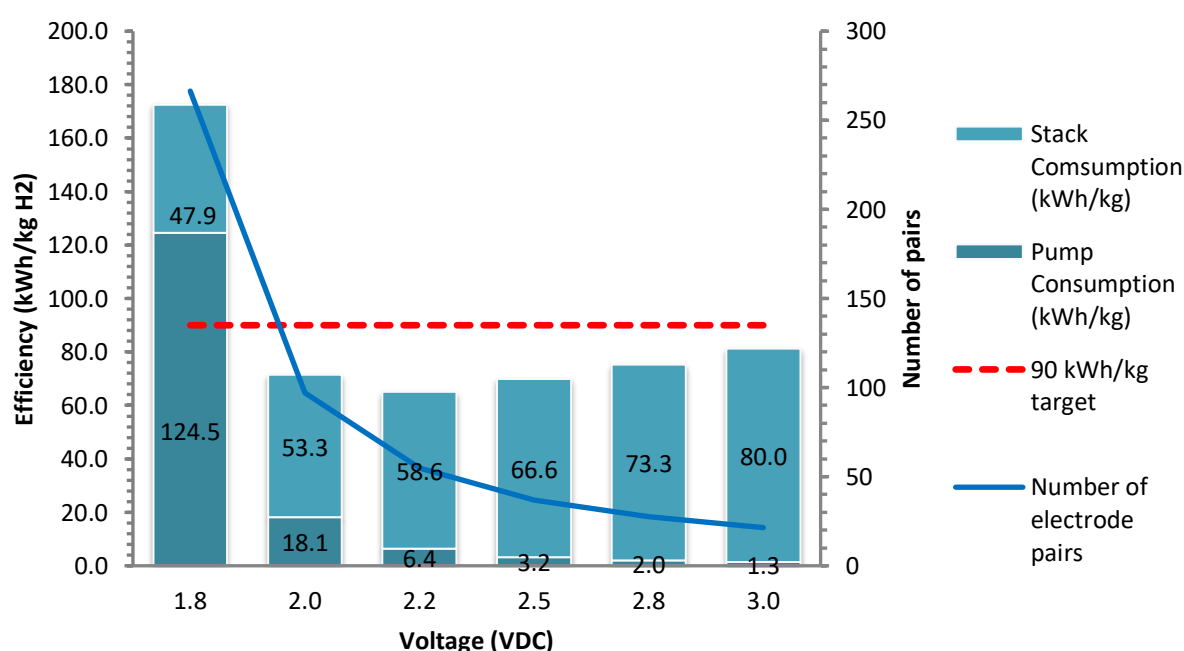


**Figure 3-15: Power consumption and stack size at  $80^{\circ}\text{C}$  for an electrolytic velocity of  $0.001 \text{ m.s}^{-1}$  at variable operating voltages.**

Figure 3-15 indicates that at a flow velocity of  $0.001 \text{ m.s}^{-1}$  the desired operating range is between 2 and 2.5 volts DC. Within this range, there is an optimal trade-off between parasitic load and stack power consumption minimising the overall power consumption per kg of hydrogen produced. For operations at 1.8 VDC to become economical, cell resistances need to be reduced and flow velocities would need to be further lowered. Although the stack power consumption at 1.8 VDC is low, the large electrode area/large number of pairs required (assuming operations with the latest/current design) results in a large pressure head and high flow requirement and hence large parasitic load. At 1.8 VDC the estimated power consumption amounts to 172 kWh/kg  $\text{H}_2$  of which the pump contributes 124 kWh/kg  $\text{H}_2$  (72%). As noted, the Bi-MCFP pilot plant experienced a low flow limit at the velocity point of  $0.001 \text{ m.s}^{-1}$ . With no drop off in gas purity being noted at this flow velocity, it is believed that further reduction in flow could be achieved with the operation of the  $5 \text{ }\mu\text{m}$  non-conductive mesh. Flow reduction and the incorporation of an effective catalyst would work towards making operations at 1.8 VDC more favourable.

Operating at 2.2 VDC results in the lowest overall power consumption of 65 kWh/kg  $\text{H}_2$  (60.61% HHV) and with an electrode area of  $350 \text{ cm}^2$  per electrode pair a total of 55 electrode pairs would be required, however, operating at 2.5 VDC with a power consumption of 70 kWh/kg  $\text{H}_2$  (56.41% HHV) a total of 36 electrode pairs would be required. It should be noted that if the outer diameter (OD) of the electrode were increased further this would result in a reduction in the number of electrode pairs, however, this would not result in a reduction in volumetric flow. Although the Bi-MCFP DEFT™ design allows for the increase in the fluid flow path, (the difference between the electrodes OD and ID) the extent to which this can be increased, still needs to be investigated.

### **3.3.4 Performance as a Function of Turndown Ratio**

The previous section (Section 3.3.3) provided an investigation for parameter selection within the realms of the latest design. It, therefore, provided the necessary conditions that are required to produce a system with a 3 - 5 kg/day  $\text{H}_2$  capacity without any further design modifications to the existing setup working only with the addition of more electrode pairs. Although this investigation served a purpose, the values provided at low voltages (such as 1.8 VDC) are not representative. To operate at 1.8 VDC, the size of the electrode would need to be increased to reduce the number of electrode pairs required. The low current densities would allow for operation at a lower flow velocity hence the pump power consumption realised would be lower than that highlighted in Figure 3-15. In summary, if operating at 1.8 VDC were the immediate goal the design would be reassessed as to better suit this operating point. The pressure head and flow requirement assumptions made from observations on a 4-cell stack possibly provides a large error when

extended to a large number of cells in the stack. An investigation into the performance of DEFT™ in its current state as a function of turndown ratio provides a means of assessment that is irrelevant of the stack size, therefore, focusing on the change in hydrogen production capacity (current density change) and overall system efficiency with the change in operating potential.

Operation at 2.2 VDC was selected as the basis point for this study, as 2.2 VDC provides a near-optimal overall power consumption at a temperature of 80°C, a flow velocity of 0.001 m.s<sup>-1</sup>, an electrode area of 1.94 m<sup>2</sup> and volumetric flow-rate of 231 L/min. The study makes use of the same setup and assumptions as those highlighted in Section 3.3.3. The turndown ratio is defined as the quotient of the maximum capacity and the capacity under assessment as per Eq. 3-1, however, since operations at 2.2 VDC does not provide a maximum capacity point, but rather a preferred operating point, a turnup ratio has been defined as per Eq. 3-2. Figure 3-16 provides a performance curve as a function of turndown/turnup ratio at a 2.2 VDC basis at a flow velocity of 0.001 m.s<sup>-1</sup>.

$$\text{Turndown Ratio} = \frac{\text{Production Rate @ 2.2 VDC}}{\text{Production Rate @ 1.8 – 2.2 VDC}} \quad \text{Eq. 3-1}$$

$$\text{Turnup Ratio} = \frac{\text{Production Rate @ 2.2 – 3 VDC}}{\text{Production Rate @ 2.2 VDC}} \quad \text{Eq. 3-2}$$

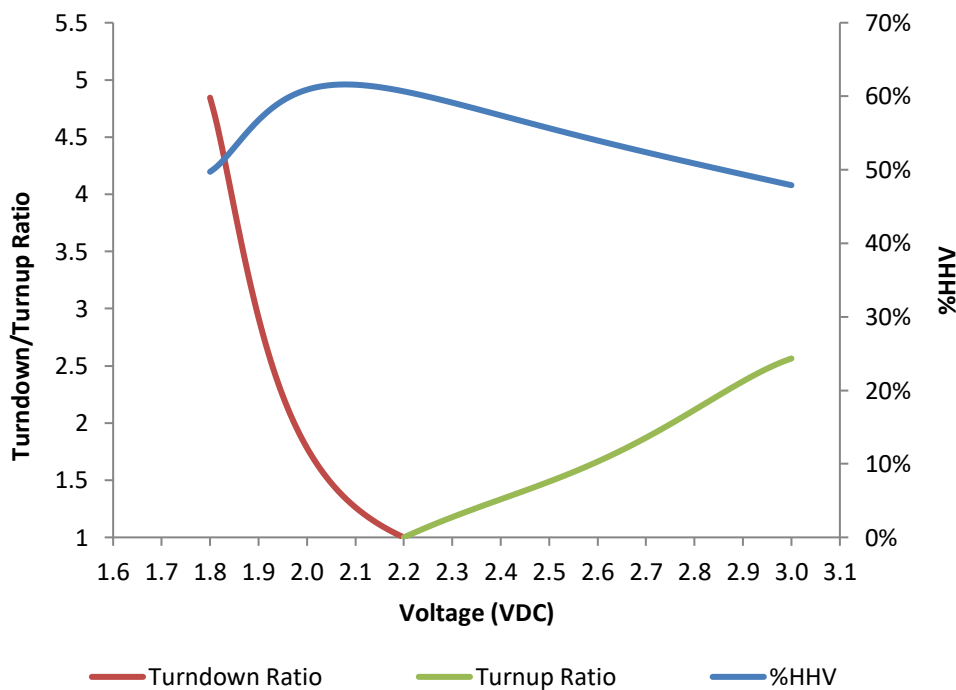


**Figure 3-16: Performance curves as a function of turndown/turnup ratio at 80°C with an electrolytic flow velocity of 0.001 m.s<sup>-1</sup>**

Figure 3-16 indicates that reducing the voltage from 2.2 to 1.8 VDC results in a turndown ratio of 4.84 thus reducing the production capacity from 5 to 1.03 kg/day H<sub>2</sub> with an efficiency of 49.7 HHV%. With an increase in voltage from 2.2 to 3 VDC a turnup ratio of 2.56 is noted with an efficiency of 48 HHV%, therefore with a 12% loss in HHV% the production rate can be increased from 5 to 12.82 kg/day H<sub>2</sub>. It should be noted that the HHV% reaches a maximum of 61% in the range of 2.1 – 2.2 VDC. This maximum value shifts further to the left of the x-axis as the flow velocity decreases. Decreasing the flow velocity to 0.0005 m.s<sup>-1</sup> shifts the maximum efficiency to 65 HHV% at 2.08 VDC.

### 3.3.5 Single Electrode Alternatives

Alternative mesh weaves have various repercussions on the active area provided along with affecting the ease for which produced gas and electrolytic solution passes through the porous structure. Higher active surface area will result in higher current densities, however, this may provide resistance for bubble passage and therefore result in increased bubble void fraction in the cell. These all influence the cell's performance. The following were assessed from available mesh options, with the available areas indicated:

- 80 µm plain dutch weave: 4.505 cm<sup>2</sup> surface area / cm<sup>2</sup> cross-sectional area
- 250 µm plain dutch weave: 4.38 cm<sup>2</sup> surface area / cm<sup>2</sup> cross-sectional area
- 485 µm plain weave: 0.74 cm<sup>2</sup> surface area / cm<sup>2</sup> cross-sectional area

Dutch weaves are regarded as ideal to use due to their high surface area per unit cross-sectional area, which ultimately would provide more area for the reaction occur on. This is desirable when considering that DEFT™ operates on the principle of electrolytic flow, and optimisation of the current density as a function of flow velocity per cross-sectional unit area would aid in reducing the required parasitic load.

It is important to take cognisance that high surface area electrodes with small pores would not be practical as gas that collects in the electrodes frontal and interstitial surfaces would negatively affect the current density and product gas quality. A balance is therefore essential between a flow friendly electrode design and high surface area configuration. IV data for the operation of the various mesh types is provided in Figure 3-17.

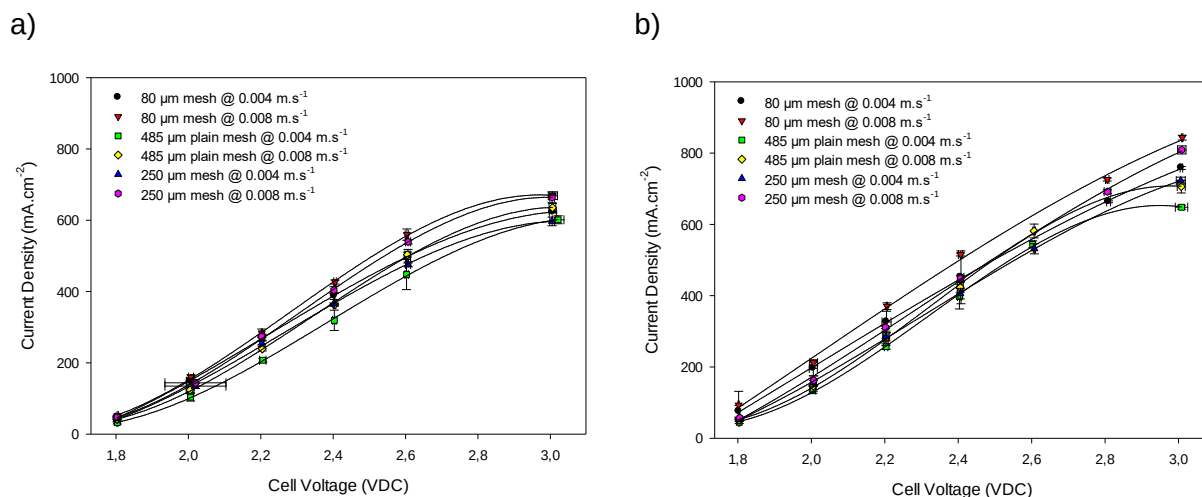


**Figure 3-17: Polarisation curve for the Bi-MCFP reactor for (a) 50°C and (b) 60°C, as a function of a single layer of specified configuration, 25 µm non-conductive mesh, an electrode gap of 2.5 mm, 30% KOH**

Figure 3-17 demonstrates that the dutch weave mesh types do indeed produce the best performance. The dutch weave electrode types exhibit similar performance to one another with the 80 µm producing only marginally better results. What was intriguing is that the plain weave has a significantly lower geometric area, however, it is capable of operating at performances only slightly lower than the dutch weave alternatives. The surface area-based current density was, hence, substantially greater implying efficient use of most of the electrode surface. The compromise may be the loss of active area due to bubble formation on the electrode surface. Dutch weaves would, however, be the preferred choice for large stack designs due to their structural stability.

### 3.3.6 Double Layer Electrode Alternatives

Prior research and development noted that having two mesh layers on top of one another for both the anode and cathode, provides up to an additional 40% improvement in current densities at set cell potentials [1], [22]. This is solely based on the additional area provided employing a double layer, and it was noted that adding a third layer added 9% to the current density at set cell potentials which implies that the third layer would not be cost-effective. Multiple configurations were attempted in this investigation making use of different porous nickel layers. The results of such are provided in Figure 3-18.

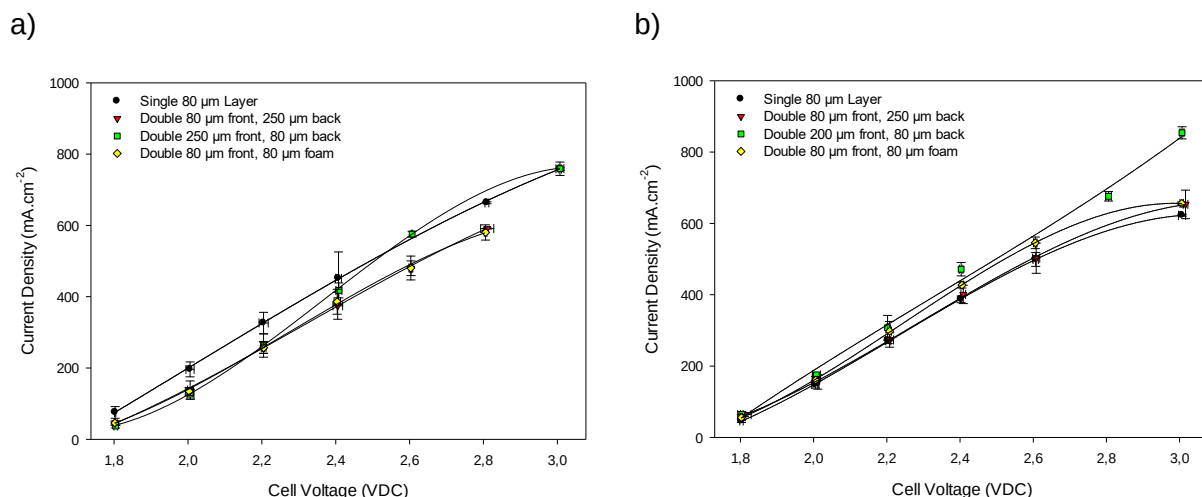


**Figure 3-18: Polarisation curve for the Bi-MCFP reactor for (a) 50°C and (b) 60°C, as a function of a double layer of specified configuration, 25 µm non-conductive mesh, an electrode gap of 2.5 mm, 30% KOH, 0.004 m.s<sup>-1</sup>.**

The results portrayed in Figure 3-18 communicate the opposite of what would be expected when it comes to enhancing the electrode area. Why a single layer of mesh performed similarly and, in some instances, better, could be explained by the drastic reduction in flow. Less flow would imply that it is harder to remove the bubbles from the surface of the electrode, and between mesh layers, which increases the residence time of the gas bubbles and thereby increases cell resistance. In addition, an additional layer of material would account for a significant increase in backpressure. Purge gas entering into the electrode gap was observed, which implied that more flow would be needed to create the separation of gases if multi-layered electrodes were to be utilised, however, the increase in cell performance would not counterbalance the load required for pumping. Figure 3-19 extends this investigation to variable flow rates and multilayer electrode configurations.

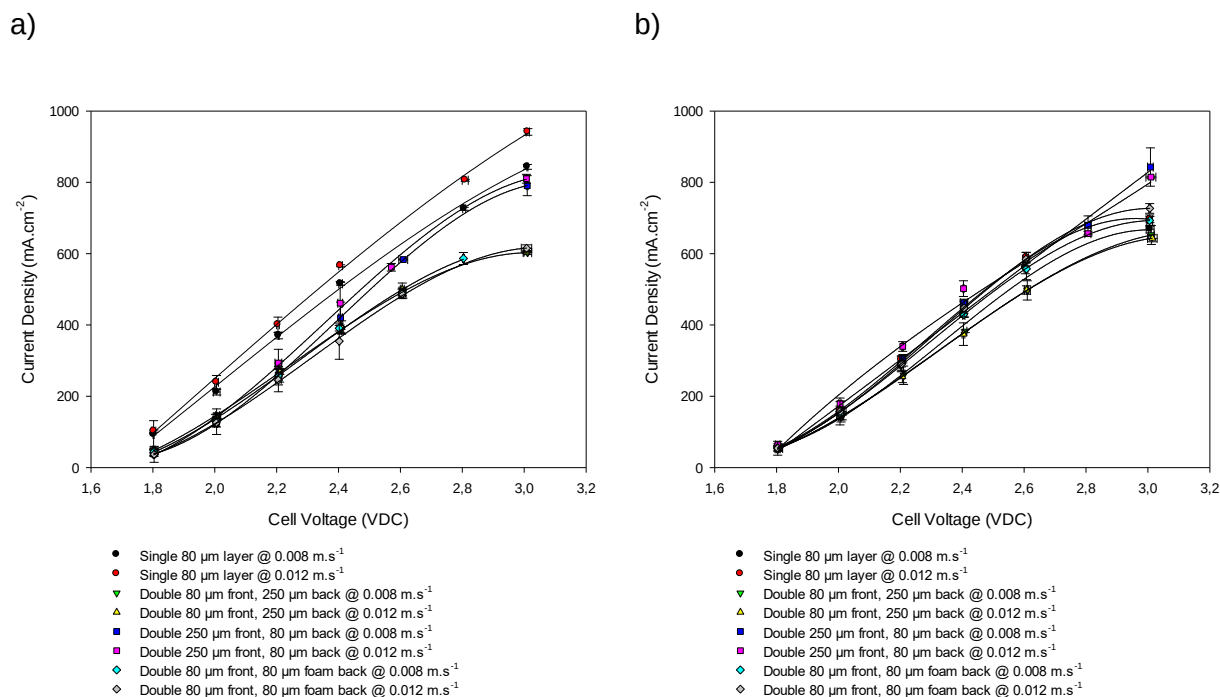


**Figure 3-19: Polarisation curve for the bi-MCFP reactor for (a) 50°C and (b) 60°C, as a function of a double layer of specified configuration, 25 µm non-conductive mesh, an electrode gap of 2.5 mm, 30% KOH, flow velocity of 0.008 m.s<sup>-1</sup> & 0.012 m.s<sup>-1</sup>.**

At greater flows, the effect of bubbles covering the surface of the electrode can be observed clearly. The single-layer can be seen to outperform all double porous layers at 50°C, however, for 60°C some of the double layers start to outperform the single layer of mesh. A combination of the decrease in solution viscosity and increase in solution velocity enhances the performance of some of the double layers above that of the single layer. The increase, however, remains marginal in contrast to the single layer of mesh, and hence the additional cost would not justify the incremental performance gains, hence, with the latest design, a single layer would represent a simplistic and reliable approach.

### 3.3.7 Electrolyser Durability

The Bi-MCFP electrolyser stack was analysed for durability for just over 300 hours at a constant current density of 500 mA.cm<sup>-2</sup>, flow velocity of 0.002 m.s<sup>-1</sup> and temperature of 60°C. The electrolytic solution was maintained at a constant concentration by monitoring the liquid level of the solution while additionally calculating the amount of water consumed with time. Polarisation data throughout this test is depicted in Figure 3-20.

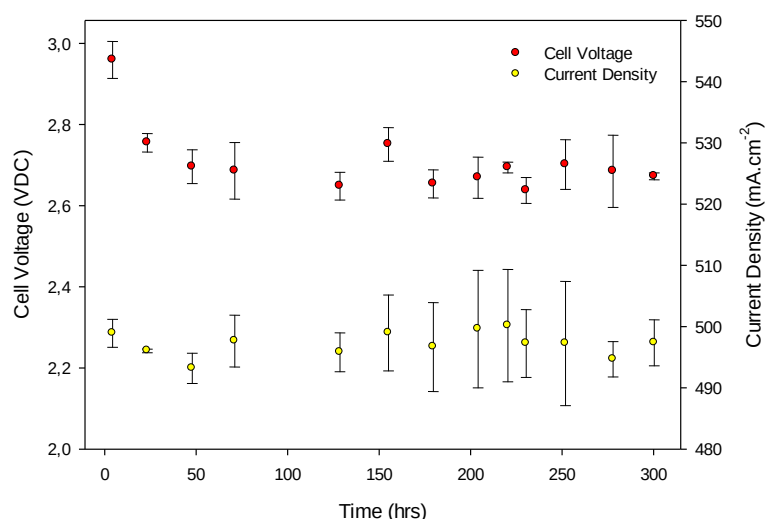


**Figure 3-20: Current density and cell voltage versus time for the Bi-MCFP stack containing 4 electrode pairs operating at 500 mA.cm<sup>-2</sup>, 30% KOH, electrode gap of 2.5 mm, 0.002 m.s<sup>-1</sup>, 5 µm non-conductive layer, and a temperature of 60°C**

Figure 3-20 illustrates the cell voltage at constant current density. Current density was maintained within the region of 500 mA.cm<sup>-2</sup> with limited error associated. Observations concerning the cell voltage note that the initial starting cell voltage is close to 3 VDC. The cell potential is then seen to taper off and stabilise between 2.753 – 2.65 VDC at a current density of 500 mA.cm<sup>-2</sup> with an error range of  $\pm 10$  mA.cm<sup>-2</sup>. Upon initiating the durability analysis of pure nickel electrodes, the surface of each electrode was etched in 17% HCl solution for 4 minutes at an anodic current density of 500 mA.cm<sup>-2</sup>. This yielded a chemically roughened surface suitable for gas nucleation due to the presence of multiple irregularities. The possible cause into the high initial starting voltage may have been due to the anodic process carried out to etch the surface. A subsequent oxidised surface may have formed, which may have represented a limiting surface for the hydrogen evolution reaction on the cathode. Secondly, over time the surface was deposited with dendritic structures containing majority iron as represented in the SEM image provided in Figure 3-21. This may have changed the kinetic nature of the electrodes surface.

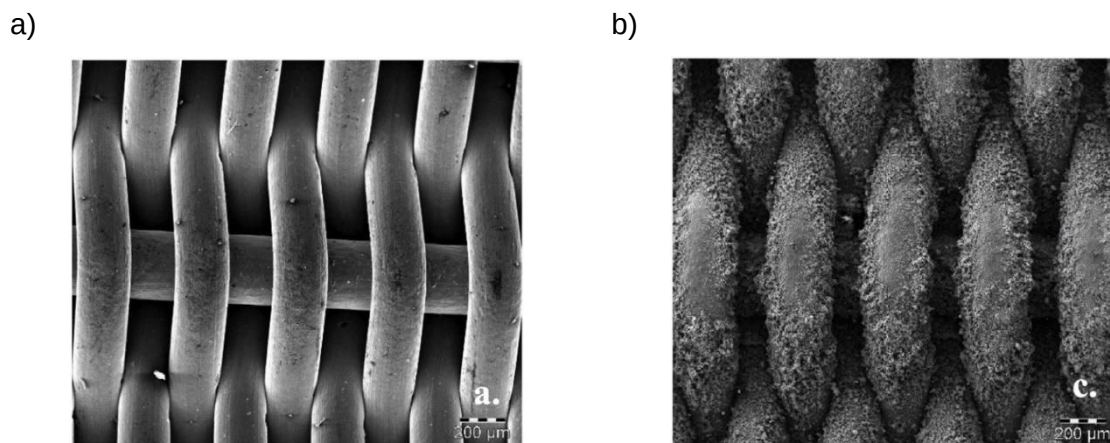


**Figure 3-21: (a) smooth surface (untreated) of pure nickel 80  $\mu\text{m}$  dutch weave and (b) dendritic iron formations on the surface of the cathodic electrode (Extracted from [1] – Permission Granted in Appendix G)**

Despite the oxygen evolution reaction, representing the limiting reaction, the collection of structures on the hydrogen electrode produces some benefit to reducing the overpotential of the water electrolysis reaction. It was found that the accumulation of this coating reaches a threshold where the coating thickness ceases to increase. Particles seem to break off from the electrode and subsequently find their way to the process strainer. For the proposed 3 - 5 kg/day  $\text{H}_2$  system, a reputable strainer system would therefore be imperative to add to the system to remove these particles. Online gas purity for hydrogen and oxygen was additionally monitored with time during the durability performance analysis.

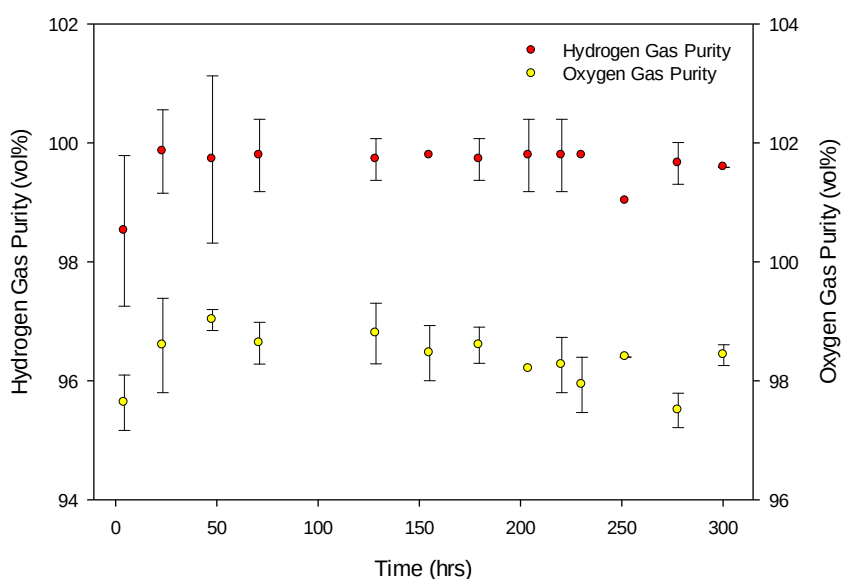


**Figure 3-22: Hydrogen and oxygen gas purity versus time for the bi-MCFP stack containing 4 electrode pairs operating at  $500 \text{ mA}\cdot\text{cm}^{-2}$ , 30% KOH, electrode gap of 2.5 mm,  $0.002 \text{ m}\cdot\text{s}^{-1}$ ,  $5 \mu\text{m}$  non-conductive layer, and a temperature of  $60^\circ\text{C}$**

Upon analysis of Figure 3-22, it is clear that the hydrogen gas produced achieved the desired gas purity being above the 99.5 vol% mark. Oxygen appears to have not performed as well, however, a reading range of 98.41 vol% for oxygen does not correspond to the oxygen purities obtained in the independent laboratory assessment in Table 3-4. The value, hence, displayed by the device appears to be slightly lower than the true value. The hydrogen reading, however, read by the device seems to match the purities provided by the independent laboratory analysis. The purity readings were generally characterised with negligible fluctuations. The DEFT™ configuration incorporating the modification appears to reliably produce gas of the adequate purity in line with current alkaline systems.

### 3.4 Conclusion

Modifications to the design of the electrode (circular to ring-shaped) and the incorporation of a non-conductive mesh (minimising gas cross-over and the effects of the meniscus) have allowed for a 75-fold reduction in electrolytic fluid velocity. At a flow velocity of  $0.001 \text{ m.s}^{-1}$ , operating temperature and voltage of  $80^\circ\text{C}$  and 2.2 VDC respectively, the parasitic load amounts to 4.6% of the overall power consumption. At these operating conditions, an efficiency of 60.6 HHV% is achieved relating to a potential overall power consumption of 65 kWh/kg  $\text{H}_2$ . It is expected that with further developments in the near term the overall efficiency can be improved to approach 70 HHV%. Further tests involving reduced flowrates, larger flow paths, higher operating temperatures, catalyst incorporation and CFD simulations focused on flow optimisation will form the pathway to achieving higher overall efficiency.

**Table 3-6: Comparison of performance data of the Bi-MCFP vs MCFP prototype**

| Parameter                                                           | Bi-MCFP Prototype | MCFP prototype [1] |
|---------------------------------------------------------------------|-------------------|--------------------|
| Voltage (VDC)                                                       | $2.00 \pm 0.01$   | 2.0                |
| Temperature ( $^\circ\text{C}$ )                                    | 60                | 60                 |
| Current Density ( $\text{mA.cm}^2$ )                                | $104 \pm 5.9$     | 578                |
| Flowrate velocity ( $\text{m.s}^{-1}$ )                             | 0.001             | 0.075              |
| Required cathodic electrode area for 5 kg/day $\text{H}_2$ capacity | 5.3               | 0.96*              |
| Flowrate required for 5 kg/day $\text{H}_2$ capacity                | 635               | 8 625*             |
| Pump and stack energy consumption                                   | 71.4              | 144.2*             |
| % parasitic load                                                    | 25.3              | 63*                |

\* Calculated under the assumptions listed in Section 3.3.3

The incorporation of a non-conductive mesh has shown that the DEFT™ principle is now capable of scale-up to enhanced gas production rates. The finalised principle is, more fundamentally, capable of significant flow reductions without sacrificing gas purities with the added benefit of greatly reducing the purge gas production emanating from the electrode gap. It is apparent that with the 110 mm electrode size a significant number of electrode pairs would be required to fulfil the production requirement of a 3 - 5 kg/day H<sub>2</sub> system. An electrode pair incorporating substantially more electrode area, but for a similar cell volume, would therefore be ideal in reducing the length of the reactor stack. An electrode scale-up to a flow path of 65 mm (230 mm OD) will provide the next step for scale-up assessment. A schematic of this electrode is provided in Figure 3-23.

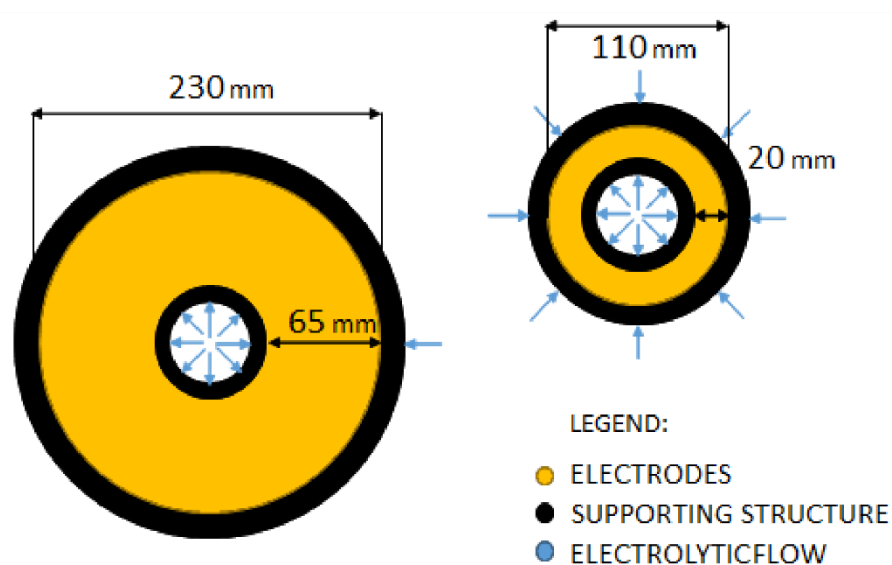


**Figure 3-23: Schematic showing potential electrode scale-up.**

From this initial study the following components will form the basis of further assessments.

1. Central inlet only as no substantial benefit was noted from the dual inlet. The dual inlet, however, adds a substantial area to the electrode housing. Consequently, utilising the single central injection manifold would work to reduce the electrode to housing area ratio.
2. The 5  $\mu\text{m}$  non-conductive layer. Further flow reductions are still required. The 5  $\mu\text{m}$  non-conductive mesh proved to exhibit the most potential in terms of reducing flow while still maintaining gas purities and mitigating purge gas. The 5  $\mu\text{m}$  mesh showed similar performance to the 10  $\mu\text{m}$  mesh, hence, has been selected as a means to minimise the overall system power consumption
3. With regards to the mesh type little improvement was observed with the incorporation of multi-layered mesh electrodes (and with its associated CAPEX increase), and therefore a single 80  $\mu\text{m}$  Ni 200 plain dutch weave will be utilised in further investigations.

## CHAPTER 4 - COMPUTATION FLOW DYNAMICS INVESTIGATION

### 4.1 Overview

A Computational Fluid Dynamics (CFD) analysis was completed on the Hydrox Holdings Bi-MCFP Electrolyser design. Various fluid injection configurations, along with the presence and absence of porous layers (electrodes and non-conductive mesh) in the reactor were simulated to see the resulting effect on the fluid flow and velocity profiles throughout the reactor. Areas of interest in the reactor's fluid flow profile are as follows:

1. How the fluid velocity changes through the total length of the injection chamber, and the resultant effect on the velocity of the fluid in contact with the electrode.
2. The behaviour of the fluid at the inlet to the electrodes.
3. The distribution, and level of entrainment of the fluid in the electrode area.

The ideal operation of the Bi-MCFP electrolyser would involve a well-distributed flow throughout the electrolyser and a relatively uniform velocity profile at the electrode inlets. This shows that each electrode pair receives fluid and provides an even distribution across the electrodes. This is indicative of good contact between the electrolyte and all of the electrodes, which increases the overall efficiency of the reactor and associated gas separation efficiency. Special attention was paid to the purge chamber to ensure no purge gas was recycled/re-introduced into any of the cells along the reactor's length.

The CFD investigation served to provide an approximated analysis of the expected flow patterns within a Bi-MCFP electrolyser stack. An approximation of the distribution of flow across the electrode face of the current configuration was made base on the stack in a state of no gas production. This was achieved by allowing SolidWorks Flow Simulation to mimic the presence of a porous structure such as the monofilament 5  $\mu\text{m}$  nylon mesh used within the Bi-MCFP electrolysis stack. The pressure drop across this material can, therefore, to some degree, be a contributing factor in the development of fluid velocity and pressure profiles within each electrode pair and the electrolyser stack. It is still acknowledged, however, that CFD results are at best a conjecture of what can be expected within a realistic application. It is an informative start when considering prototype development or improvement, in retrospect to implementing rapid prototypes, and can result in saving cost and time. SolidWorks Flow Simulation 2016 has therefore been selected as a tool to deduce the results. The following operational scenarios form part of this assessment.

1. Injection from **one end** of the reactor stack with **no NC mesh**; gas outlets terminate at **alternate ends**.
2. Injection from **both ends** of the reactor stack with **no NC mesh**; gas outlets terminate at **alternate ends**
3. Injection from **both ends** of the reactor stack **with NC mesh**; gas outlets terminate at **alternate ends**.
4. Injection from **one end** of the reactor stack **with NC mesh**; gas outlets terminate at the **same end of the reactor**.
5. Injection from **both ends** of the reactor stack **with NC mesh**; gas outlets are **open from both ends**.

## 4.2 Model Definition

### 4.2.1 Bi-MCFP Reactor Design

The CFD simulations were based on the latest revision of the Bi-Mono-Circular-Filter-Press (Bi-MCFP) electrolyser design. This included the suggested design modifications listed in Section 3.4. This reactor is comprised of 36 electrode pairs, with electrodes having an outer diameter of 220 mm and an inner diameter of 90 mm. A 5  $\mu\text{m}$  non-conductive mesh is used between paired electrodes to prevent gas formation on the frontal electrode face, inhibiting gas formation within the electrode gap, and allowing for lower flow rates required for effective gas separation. The injection configuration comprises the central injection chamber. Bi-phase (gas and electrolyte) outlets run above the injection chamber and are off-centred. There is another chamber above the injection chamber that acts as a purge outlet. This accounts for any impurities or accumulation within the system. The model employed, of a single cell, can be seen in Figure 4-1.

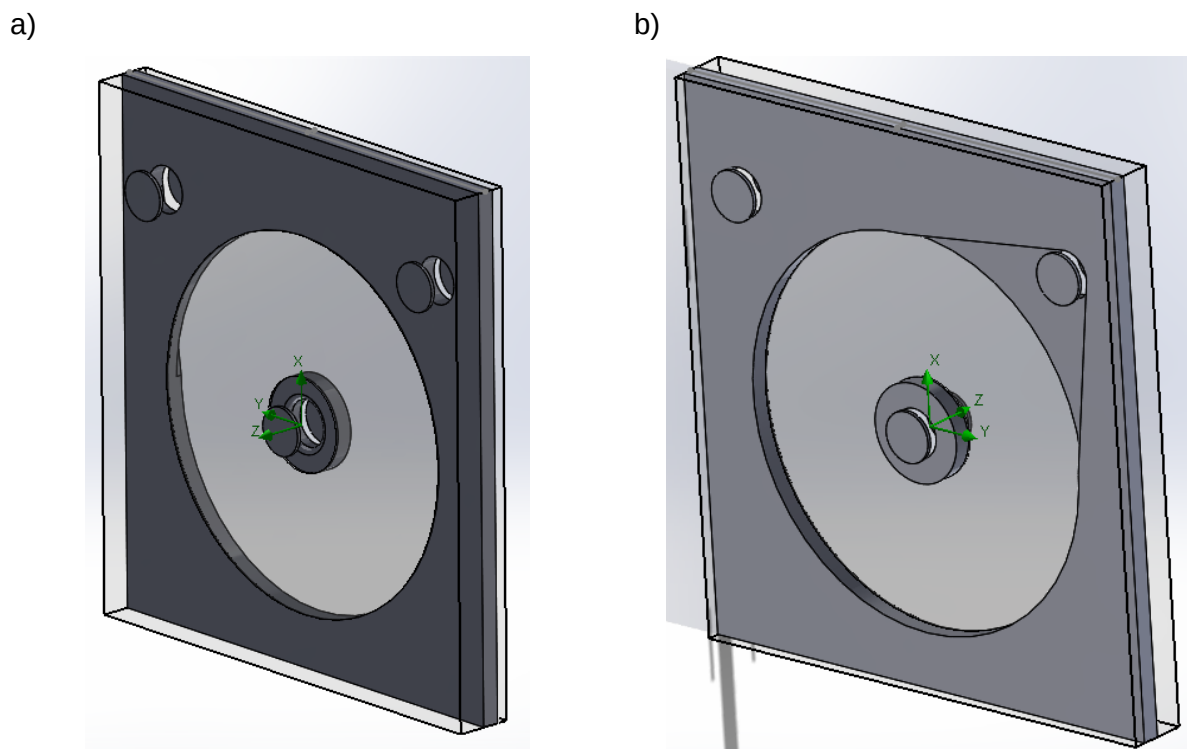


**Figure 4-1: a.) front view and b.) rear view of the current circular approach to DEFT™ electrolysis simulation model**

As a summary, this configuration makes use of a ring-shaped electrode with the following specifications:

- a. Outer diameter: 220 mm
- b. Inner Diameter: 90 mm
- c. Electrode surface area: 352 cm<sup>2</sup>
- d. Electrode Flow Path: 65 mm
- e. Electrode Gap: 2 mm
- f. Main electrolyte feed diameter: 40 mm
- g. Collection chamber exists diameter: 40 mm

Along with the above specifications, simulations were completed at a mesh rating of 5  $\mu$ m aperture.

#### **4.2.2 SolidWorks Flow Simulation Technical Reference**

Flow simulators work to solve the Navier-Stokes equations, which are a set of partial differential equations used to describe the motion of viscous fluids. They consist of equations formulated from conservation laws of mass, momentum, and energy. The equations are coupled with fluid

state equations which define the physical characteristics such as fluid density, viscosity, and thermal conductivity etc.. Flow Simulation can predict both laminar and turbulent flow regimes. In engineering, the majority of problems encountered will be turbulent in their regime, and hence the Favre-averaged Navier-Stokes equations are solved where time-averaged effects of the flow turbulence on the flow parameters are considered [103].

Flow simulation additionally solves or simplifies models for flow-through porous media, by treating the porous media as distributed resistances to fluid flow. The hydraulic resistance contributed by porous media is defined by the following equation as represented in the Navier-Stokes equation as per Eq. 4-1 [103],

$$F = k\rho v \quad \text{Eq. 4-1}$$

where  $k$  is the resistance vector of the porous media,  $\rho$  is the solution density and  $v$  is the flow velocity of the liquid. The resistance vector can be determined by Eq. 4-2 [103],

$$k = \frac{-\nabla P}{\rho v} \quad \text{Eq. 4-2}$$

where  $\nabla P$  is the pressure gradient and can be expressed as per Eq. 4-3 [103],

$$\nabla P = \frac{\Delta P}{l} \quad \text{Eq. 4-3}$$

where  $l$  is the linear solution path distance through the porous medium and  $\Delta P$  is the pressure drop across the frontal and rear faces of the material. To define  $k$ , all factors need to be defined empirically first, as per Eq. 4-4 [103],

$$k = \frac{A \cdot v + B}{\rho} \quad \text{Eq. 4-4}$$

where  $v$  is the fluid velocity,  $A$  and  $B$  are constants,  $\rho$  is the fluid density. Here, only  $A$  and  $B$  are specified since  $v$  and  $\rho$  are calculated or defined in the model. A means of defining the constants represented in Eq. 4-4 was devised. By equating Eq. 4-4 with Eq. 4-2 and simplifying the expression yields a quadratic equation, Eq. 4-5 [103].

$$-\nabla P = Av^2 + Bv \quad \text{Eq. 4-5}$$

Creating a geometric model of the 5  $\mu\text{m}$  monofilament mesh within SolidWorks, along with running simulations for a 30% potassium hydroxide solution with density references to a temperature of 20°C and 1 atm, as a function of solution flow velocity, a plot can be obtained of solution velocity versus pressure gradient. By plotting for a quadratic function with the intercept equal to zero would allow for the  $A$  and  $B$  constants within Eq. 4-5 to be solved for said conditions. The 5  $\mu\text{m}$  mesh

model, Figure 4-2, was generated to simulate the pressure drop of a 30% solution of potassium hydroxide flowing through it at variable flow velocities, similarly, a model was additionally created for a 5  $\mu\text{m}$  medium.

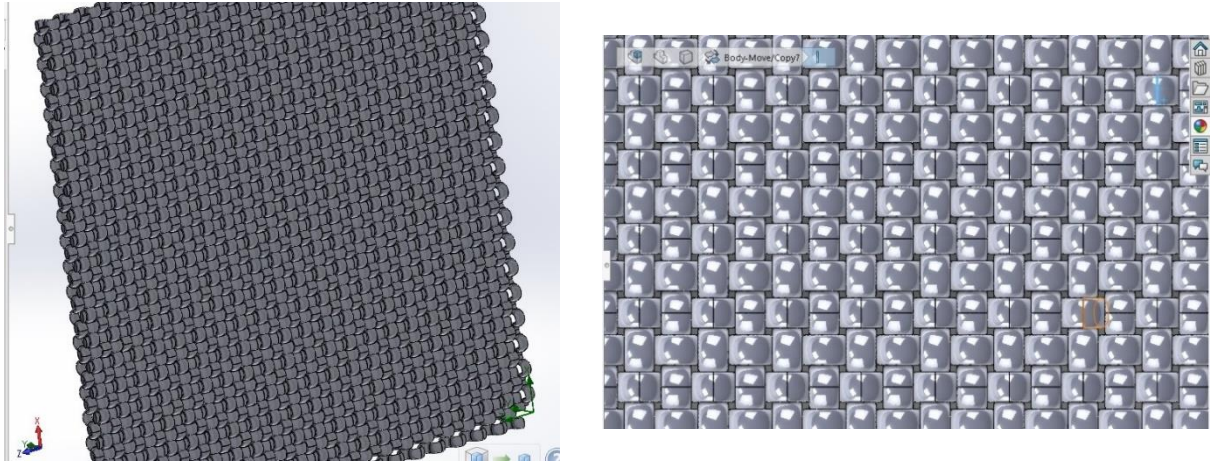


**Figure 4-2: 5  $\mu\text{m}$  nylon monofilament mesh model**

Performing a CFD analysis for the material illustrated in Figure 4-2 for a flow velocity range of  $0.00001 - 0.01 \text{ m.s}^{-1}$ , the following plots were generated along with their trend lines setting the intercept equal to zero.

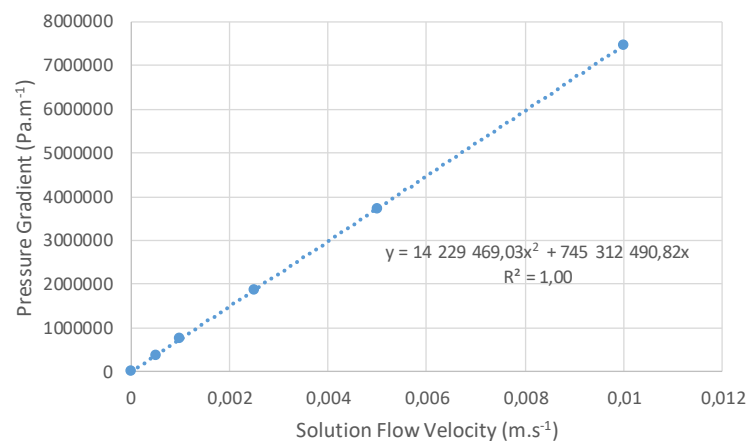


**Figure 4-3: Solution flow velocity versus pressure gradient for a 5  $\mu\text{m}$  monofilament mesh**

By extracting the A and B constants from the plots, depicted in Figure 4-3, the data can be used together with the solution properties (density and viscosity) to simulate the porous media used within the present DEFT™ system. The type of porous medium additionally also needs to be defined within SolidWorks [103]:

- Isotropic (i.e., the medium permeability is independent of direction),
- Unidirectional (i.e., the medium is permeable in one direction only),
- Axisymmetrical (i.e., the medium permeability is fully governed by its axial and transversal components concerning a specified direction),
- Orthotropic (i.e., the general case, when the medium permeability varies with direction and is fully governed by its three components determined along three principal directions).

The porous material for the following simulations has been modelled as a unidirectional porous medium due to the woven nature of the monofilament mesh.

### 4.3 Results and Discussion

#### 4.3.1 Configuration 1

This model simulates the reactor with a single injection and terminating outlets configuration. Porous media was not used in the model. The velocity profile, depicted in Figure 4-4 and Figure 4-5, was generated from the CFD simulation.

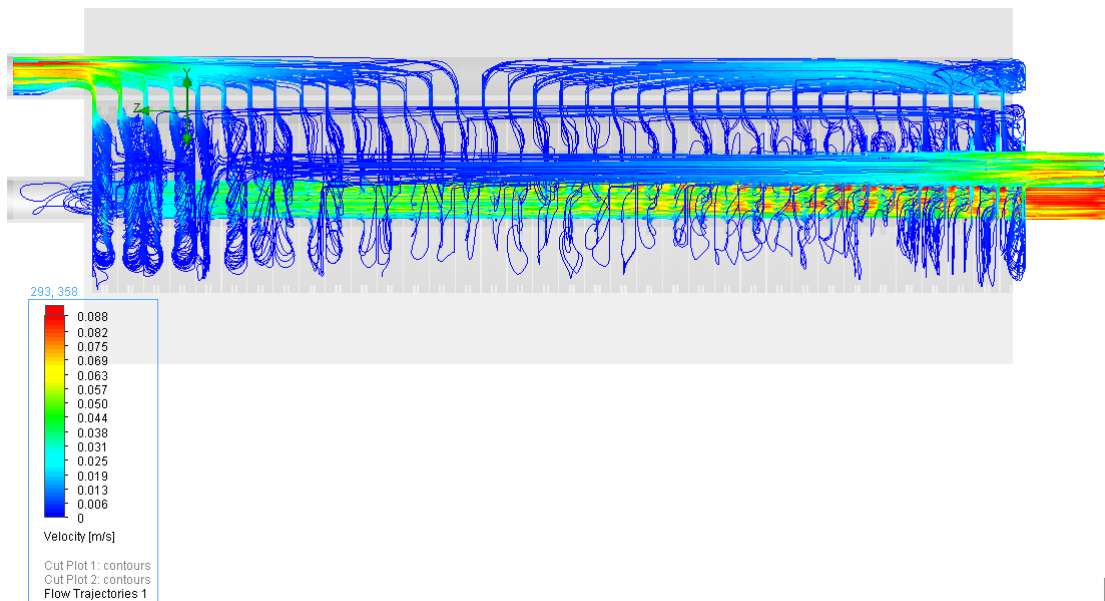


**Figure 4-4: Side view flow trajectory of configuration 1**

The velocity is maximum at the site of injection and decreases steadily along the length of the reactor, with the stream being terminated at the end of the reactor.

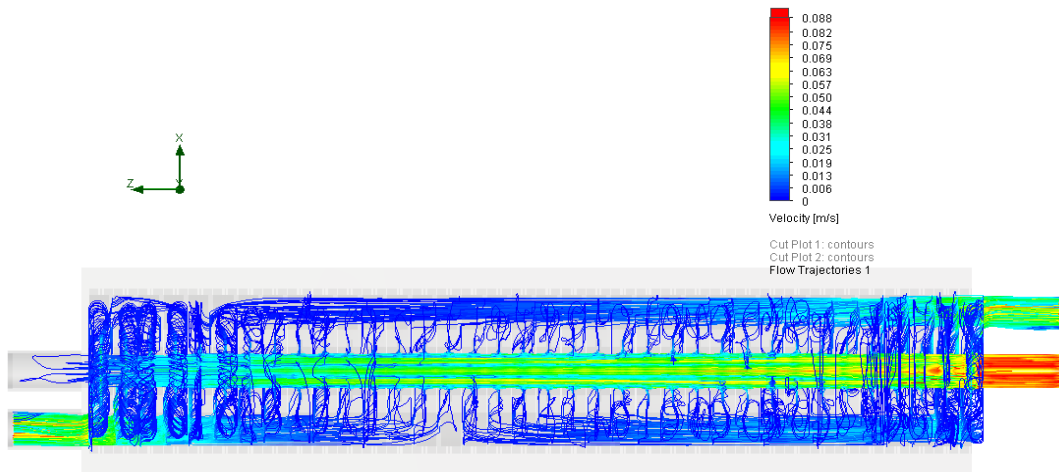


**Figure 4-5: Top view flow trajectory of configuration 1**

A conglomeration of flow lines is noted at either end of the electrolyser stack. Essentially this splits the profile within the middle region of the stack with possible recirculation noted in both former halves of the hydrogen and oxygen electrolyte outlet manifolds. With the purge, a similar result is observed within the second half of the purge manifold. This split occurs further to the left of the stack (away from the side of electrolyte injection). As the flow proceeds across the reactor the velocity gradient progressively decreases, so less fluid is distributed out of the inlet manifold to the respective cells. At the end of the reactor, the resulting back pressure from the termination of the inlet manifold causes a high-pressure point and hence a rapid drop in velocity. This contributes to the greater distribution of flow observed at the end of the reactor, as compared to that at the centre. Equal flow distribution is noted out the gas outlets on alternate ends, hence, a close to equal split between anolyte and catholyte is expected.

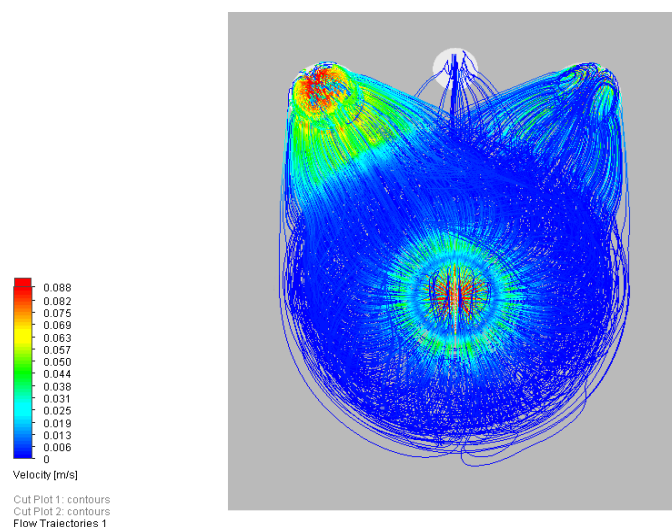


**Figure 4-6: Front view fluid trajectory of configuration 1**

Figure 4-6 shows no abnormalities in the flow along the frontal face of the electrodes. Areas of high turbulence are noted in the lower half of the stack. This is because flow entering the lower half of the electrode would ultimately need to find a path to the outlet manifold located at the upper corner of the cell.

#### 4.3.2 Configuration 2

Double injection of the electrolyte has been used in this model with gas outlets terminating at alternate ends of the reactor. No porous regions or mesh structures were included in this model. The velocity profile, depicted in Figure 4-7 and

Figure 4-8, was generated from the CFD simulation.

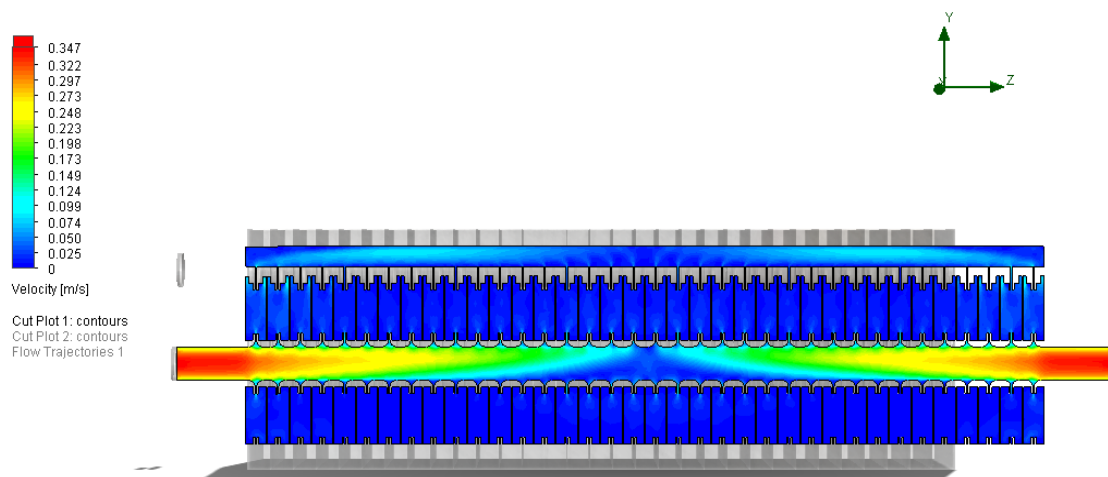


**Figure 4-7: Side sectional view velocity profile of configuration 2**

Figure 4-7 shows a side sectional view of the stack allowing velocity profiles in the inlet manifold and the purge manifold to be assessed. The flow at the injection points has the greatest velocity, as indicated by the red region in Figure 4-7. The flow initially starts as laminar, but then progressively becomes more turbulent towards the middle of the stack. It is noted that towards the centre of the stack the flow favours the upper region of the electrode. This may be due to the backpressure in the lower half of the cell providing more resistance to flow as it is furthest away from the outlet manifold. Again, the profile has been split within the cell, however, in this case, it seems to be more centralised.

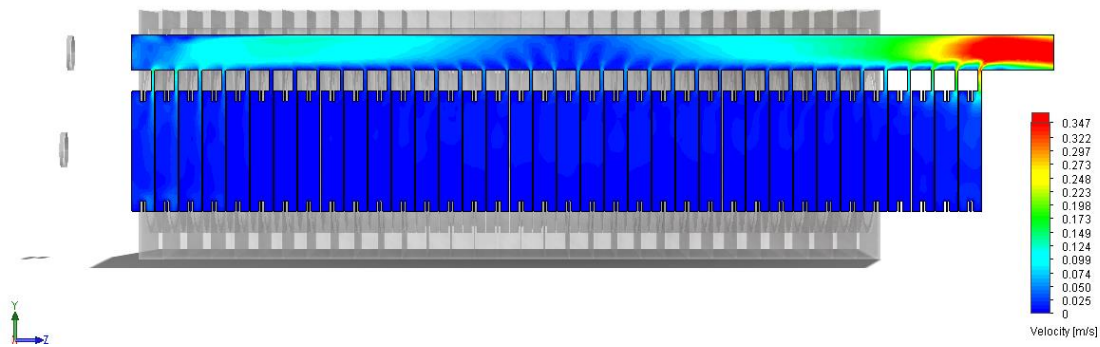


**Figure 4-8: Side view velocity profile of configuration 2**

Figure 4-8 provides a side view of the stack showing the velocity profile in a single outlet manifold. The lower velocity in the central region of the gas outlet is indicative of the split in the flow profile. Although the fluid is injected into both ends of the cell. The removal of fluid from a single side reduces electrolyte feed to the central electrode cells. Again, the possibility exists that some fluid may recycle back into the electrode cells.

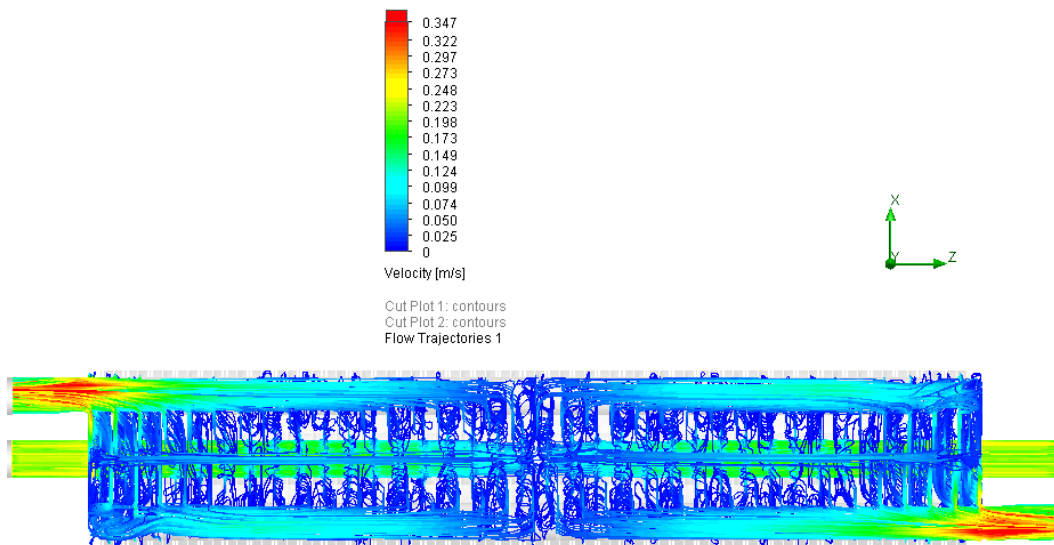


**Figure 4-9: Top view velocity profile of configuration 2**

The top view of the stack provided in Figure 4-9 further depicts the split in the flow profile across the stack. The image shows that the flow is better distributed to each electrode pair compared to what is noted with a single injection point.

### 4.3.3 Configuration 3

This model uses the double injection with alternate terminating gas outlets configuration. Standard porous media was introduced. It makes use of the same velocity profile as Configuration 2. The velocity profile, depicted in Figure 4-10 and Figure 4-11, was generated from the CFD simulation.

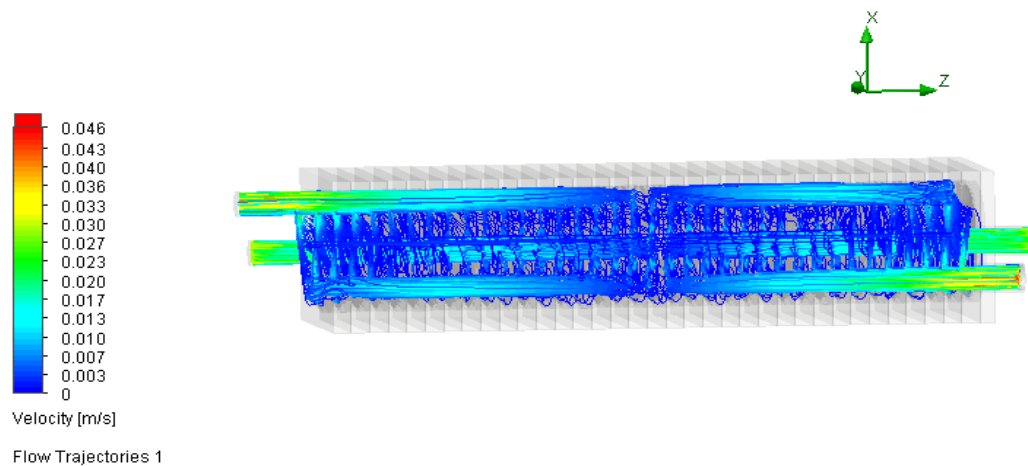


**Figure 4-10: Rotated top view for Configuration 3**

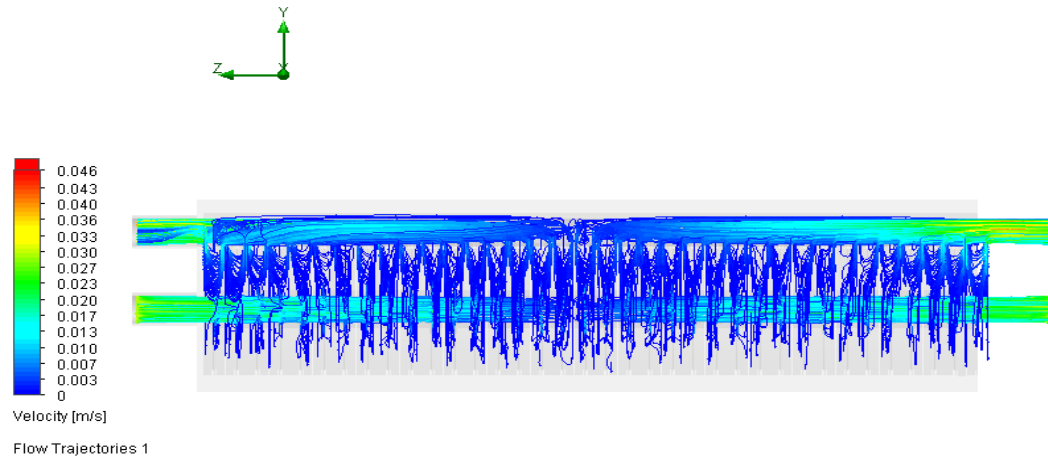


**Figure 4-11: Side view Fluid Trajectory for Configuration 3**

The porous media does not appear to result in any different or adverse phenomena when compared to Configuration 2. Flow is adequately provided throughout the inlet manifold. The increased back pressure over the electrodes caused by the porous material (non-conductive mesh) seems to result in a more uniform distribution of fluid to each electrode pair.

#### 4.3.4 Configuration 4

The flow distribution in a single injection system was not sufficient, hence the decision to use double injection, however, with the introduction of porous material in the double injection model, the flow distribution across the electrodes was noted to be more uniform, particularly in the regions between the inlets and the central region. This may indicate that using porous material would achieve improved distribution in the single injection model. The anomaly observed in previous models, in the case where there was mixing of product streams, may have occurred due to the highest-pressure points occurring at opposing ends of the reactor. This led to a symmetrical configuration of the gas outlets being adopted in this model depicted in Figure 4-12. The outlet manifolds were incorporated on the side of electrolyte injection. This was in an attempt to try to balance the pressure across the stack. The termination point of flow exhibits a high-pressure point therefore introducing the outlet manifolds (low-pressure point) on the side of flow introduction would potentially balance the flow across the stack.

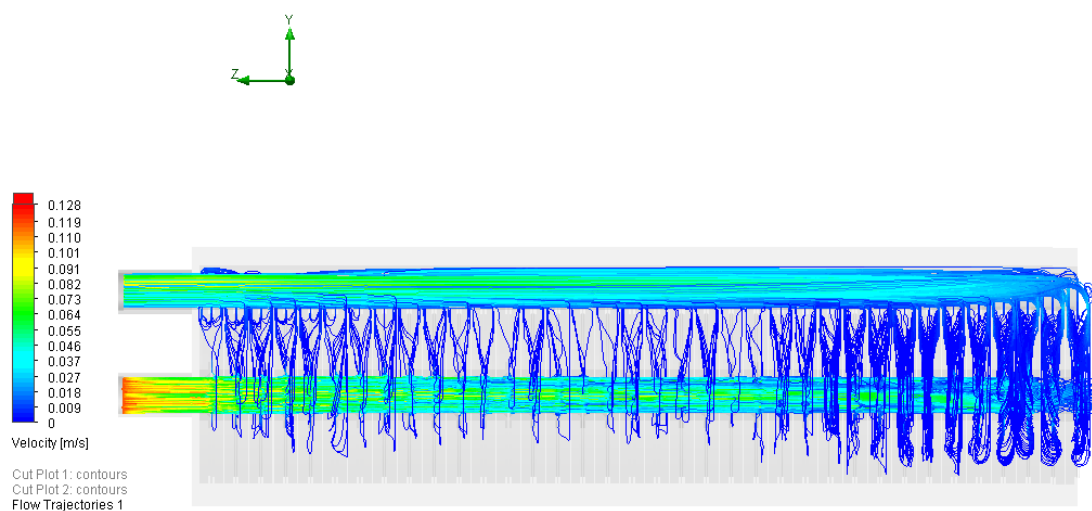


**Figure 4-12: Side view flow trajectory of configuration 4**

Having both outlet manifolds terminating on both ends does allow for the reduction/elimination of backflow in the outlet manifolds, however, the configuration notes a conglomeration of flow lines at the end of the stack (flow termination point). The flow distribution to each electrode pair is therefore not deemed adequate.

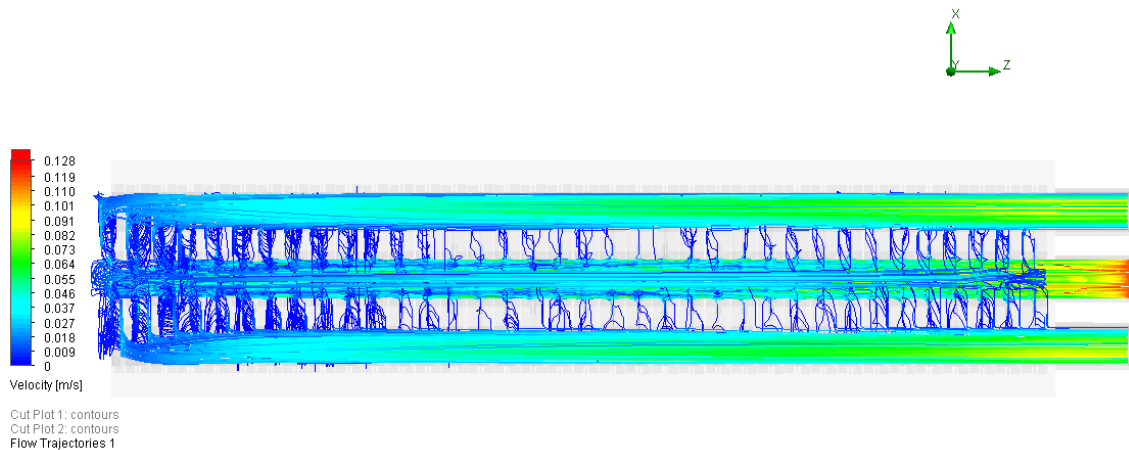


**Figure 4-13: Top view flow trajectory of configuration 4**

Further noted by the top view velocity profile in Figure 4-13, this outlet configuration reduces the profile split and potential remixing of the outlet manifolds, however, it also leads to less flow to the electrode pairs at the point of injection.

#### 4.3.5 Configuration 5

This configuration represents a network consisting of double injection inlets with double-ended gas outlets, i.e. injection and collection from either end of the stack. With the dual injection better distribution is noted, however, the flow profile is split within the collection chambers with possible recirculation noted. With dual collection on either end of the stack, the backflow may be alleviated. Figure 4-14 provides a depiction of the flow trajectory associated with this configuration.

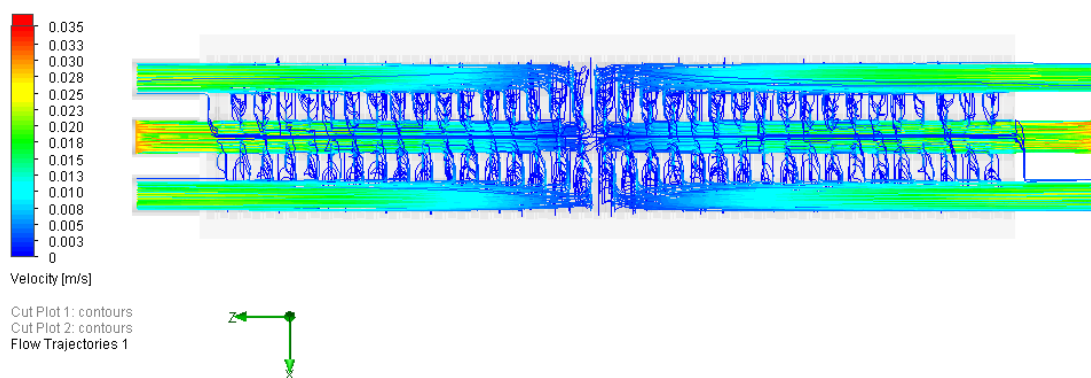


**Figure 4-14: Top view fluid trajectory for Configuration 5**

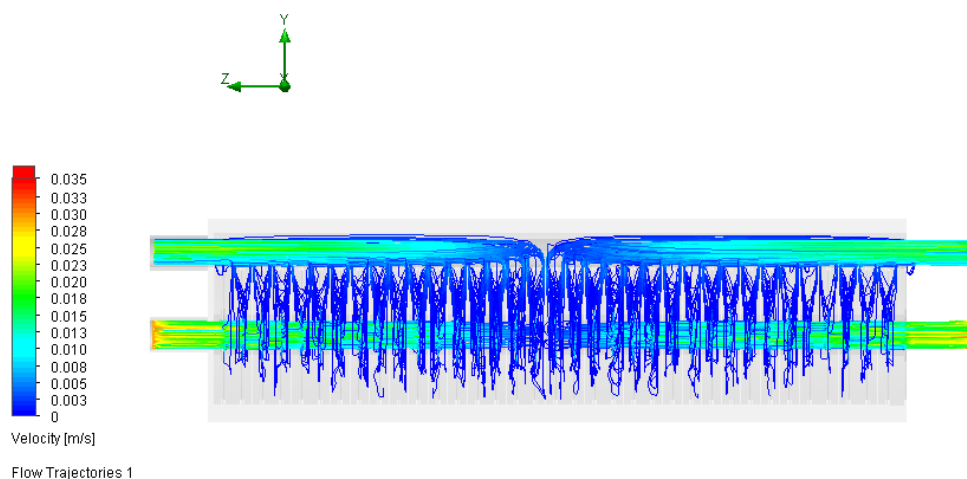


**Figure 4-15: Side view fluid trajectory for Configuration 5**

The simulation shows that this configuration achieves the desired distribution over the electrodes, whilst preventing backflow in the collection manifolds. This is because having dual outlets maintains a relatively consistent pressure gradient along the length of the reactor. Due to this consistency, and absence of backpressure in the product streams, the possibility of transfer of products between product streams is greatly reduced. This has led to the conclusion that this configuration currently provides the best configuration for the DEFT™ technology to obtain a high conversion, with product streams having a high purity.

#### 4.4 Conclusion

Initially, a single injection was used which did not achieve consistent fluid distribution for the size of the reactor simulated. This led to the development of a system with a double injection configuration that gave the desired fluid distribution when an appropriate inlet velocity was used. Backpressure in the opposingly terminated gas outlets presented a potential for the reintroduction of bi-phase solution back into the electrode cell. This was addressed by having double-ended outlets. This provided a relatively uniform pressure gradient/flow distribution along the entire length of the reactor. The observation of this study led to the development of Configuration 5 as being the configuration of choice for the scale-up to a 3 – 5 kg H<sub>2</sub> pilot.

## **CHAPTER 5 - DEFT™ TECHNOLOGY PILOT PERFORMANCE ASSESSMENT**

### **5.1 Overview**

At the conclusion of Section 3 (design and testing of the early demonstration prototype), the requirement was to extend the size of the electrode flow-path and thereby incorporating an electrode into a cell housing that would result in a higher electrode to cell housing area ratio. In addition to that two additional requirements were set for the design and commission of a 3 - 5 kg/day H<sub>2</sub> pilot.

1. The electrolyser cells needed to be powered in a series configuration, thus, allowing for the use of higher voltage lower amperage power conditioning equipment. In this way, the electrolyser stack would need to make use of bipolar plates.
2. The electrolyser stack made use of 25 mm electrode housing and injection plates, therefore, a cell pair containing 56 cm<sup>2</sup> of electrode area has a resultant thickness of 75 mm. Consequently, not only was it a goal to increase the electrode/housing area ratio but to also reduce the thickness associated with each cell to prevent the construction of an electrolyser with a substantial length.

With the modification to the design of the electrolyser, a suitable commercially viable concept balance of plant needed to be designed and constructed with the associated controls and safety checks. Plant safety was ensured through the correct selection and installation of rated EX/ATEX equipment and through the commencement of both an extensive internal and external HAZOP and safety review. On commissioning of the pilot, an electrolyser stack (of finalised design) capable of producing 3 – 5 kg/day H<sub>2</sub> was required to be installed and tested generating the necessary data to carry out a meaningful performance and techno-economic assessment.

### **5.2 Electrolyser Design Modifications**

Since the fluid dynamics is less of a critical parameter, due to the presence of the non-conductive mesh, it is believed that the design can be substantially simplified by introducing the following alterations:

1. The injection plate was removed, replaced by a recess in the electrode housing plate and a gasket defining the electrode gap.
2. The electrode housing was removed with the electrode supported in the electrode housing plate.

3. Due to the substantial reduction in electrolytic flow, the thickness of the electrode housing plates was reduced, as pressure drop through these structures would be less of a presiding influence. The plates were specified to be 16 mm in thickness compared to the prior 25 mm dimension.
4. A bipolar approach was integrated that represented a simpler, lower-cost approach in proving the electrodes with electricity. A central male and female thread were utilised to lock the anodic and cathodic cells in place (locked in place on either side of the bipolar plate).
5. Electrolyte was introduced from the inner periphery to reduce the size of the electrode housing plates.

The volume of the electrolyser was therefore substantially reduced in contrast to the current Bi-MCFP approach as illustrated in Figure 5-1. With the substantial enhancement in the cross-sectional area now available in the proposed 230 mm Bipolar Bi-MCFP reactor, the reactor volume was reduced by a factor of 6 in contrast to the 110 mm Bi-MCFP approach. This resulted in a significant reduction in the number of pairs that would be required for the 3 - 5 kg/day  $H_2$  system.

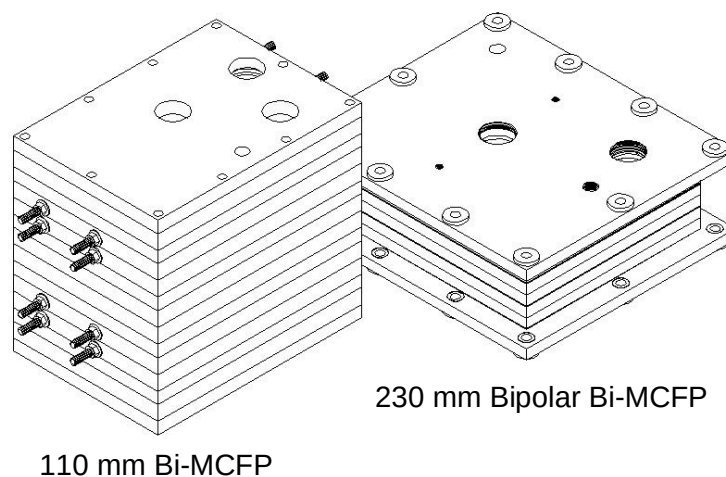


**Figure 5-1: Rendering of the 110 mm Bi-MCFP stack vs the 230 mm Bipolar Bi-MCFP stack**

A small scale stack (4 cell stack) of the 230 mm Bipolar Bi-MCFP reactor was constructed and tested on the pilot plant described and depicted in Section 3.2.3, with an image provided in Figure 5-2. The investigation surrounding this prototype will not be described in detail as the main purpose of this prototype was to de-risk the build of the 3 – 5 kg/day  $H_2$  by ensuring the modifications to the stack were successful, i.e. successful sealing of the bipolar plates and maintaining of high gas purities with the reduce size/volume of the injection chamber and the collection chamber.

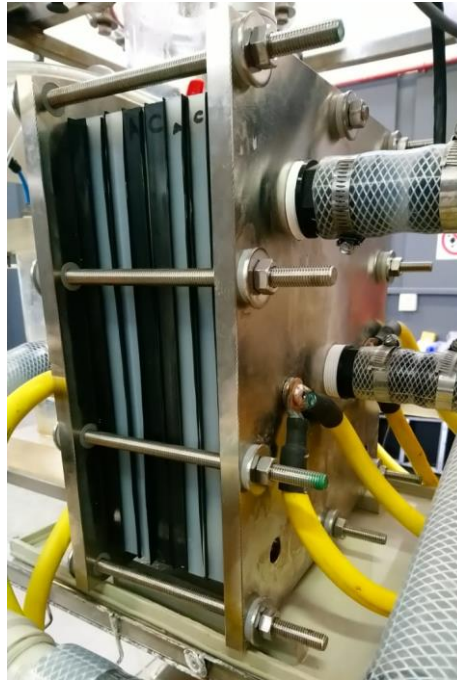
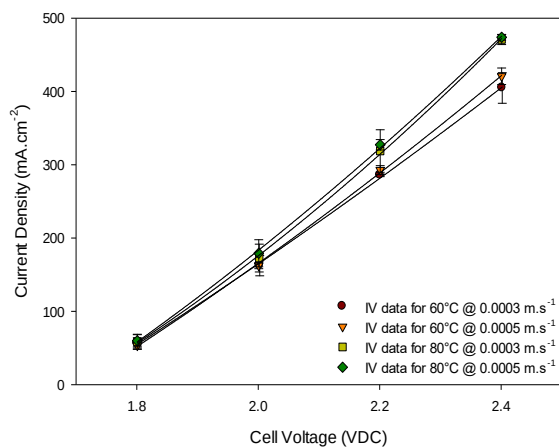


**Figure 5-2: Proof of concept 230 mm Bipolar Bi-MFCP stack**

With the stack utilising four electrode pairs, each with an area of  $352 \text{ cm}^2$ , resulting in a total electrode area of  $1407 \text{ cm}^2$ , the Bipolar Bi-MCFP reactor contains over 6 times the electrode area compared to the Bi-MCFP pilot. Consequently, operating at the lower pumping limit of the plant ( $5.5 \text{ l.min}^{-1}$ ) translates to a minimum flow velocity of  $0.0003 \text{ m.s}^{-1}$  as opposed to the Bi-MCFP resulting limit of  $0.001 \text{ m.s}^{-1}$ , hence, lower flow velocities could be assessed on this reactor prototype. IV data and gas purity data for the stack is provided in Figure 5-3.

a)



b)

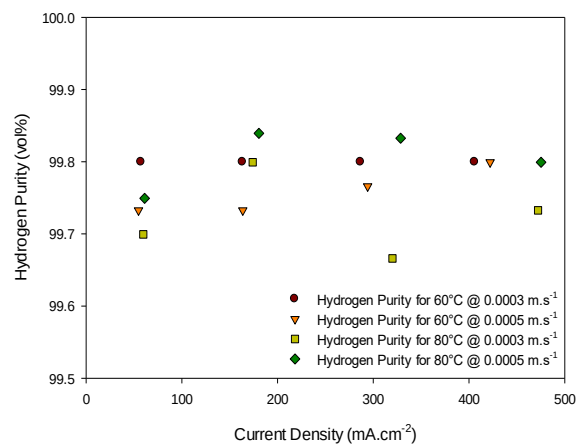


**Figure 5-3: (a) IV data for the 230 mm Bipolar Bi-MCFP stack at  $0.0003 \text{ m.s}^{-1}$  and (b) Gas purity data for the 230 mm Bipolar Bi-MCFP stack at  $0.0003 \text{ m.s}^{-1}$**

The current density observed for the 230 mm Bipolar Bi-MCFP proof of concept shows a slight improvement over the unipolar Bi-MCFP with current density points of  $122$  and  $230 \text{ mA.cm}^{-2}$  noted

at 2.0 and 2.2 VDC respectively at 60°C and at a flow velocity of 0.004 m.s<sup>-1</sup> as per Table 3-3 in Section 3.3.2. The Bipolar Bi-MCFP design noted current densities 168 and 282 mA.cm<sup>-2</sup> at similar voltages and temperature, however, operating at a slightly lower flow velocity of 0.003 m.s<sup>-1</sup>. The increase in current density is expected to be due to the added reaction area provided by the bipolar plate. At flow velocities as low as 0.003 m.s<sup>-1</sup> gas purities remained greater than 99.5 vol% H<sub>2</sub>, therefore, indicating adequate gaseous separation within the electrolyser stack that the associated electrolytic flowrate.

## 5.3 Methods and Apparatus

### 5.3.1 Finalised Reactor Design

The finalised design capitalised on the success of the initial 230 mm prototype. During the operation of this prototype, gas purities remained well above 99 vol% H<sub>2</sub> at flow velocities of 0.0003 m.s<sup>-1</sup>, as per Figure 5-3b. The design, therefore, remained the same except for an increase in electrode area/flow path. For the final 3 – 5 kg/day H<sub>2</sub> stack, an electrode with a 320 mm outer diameter and 80 mm inner diameter was selected. This resulted in a total cathodic electrode area of 754 cm<sup>2</sup> per cell. As noted, the final stack design is as per the 230 mm Bipolar Bi-MCFP design. A schematic of this design is provided in Figure 5-4.

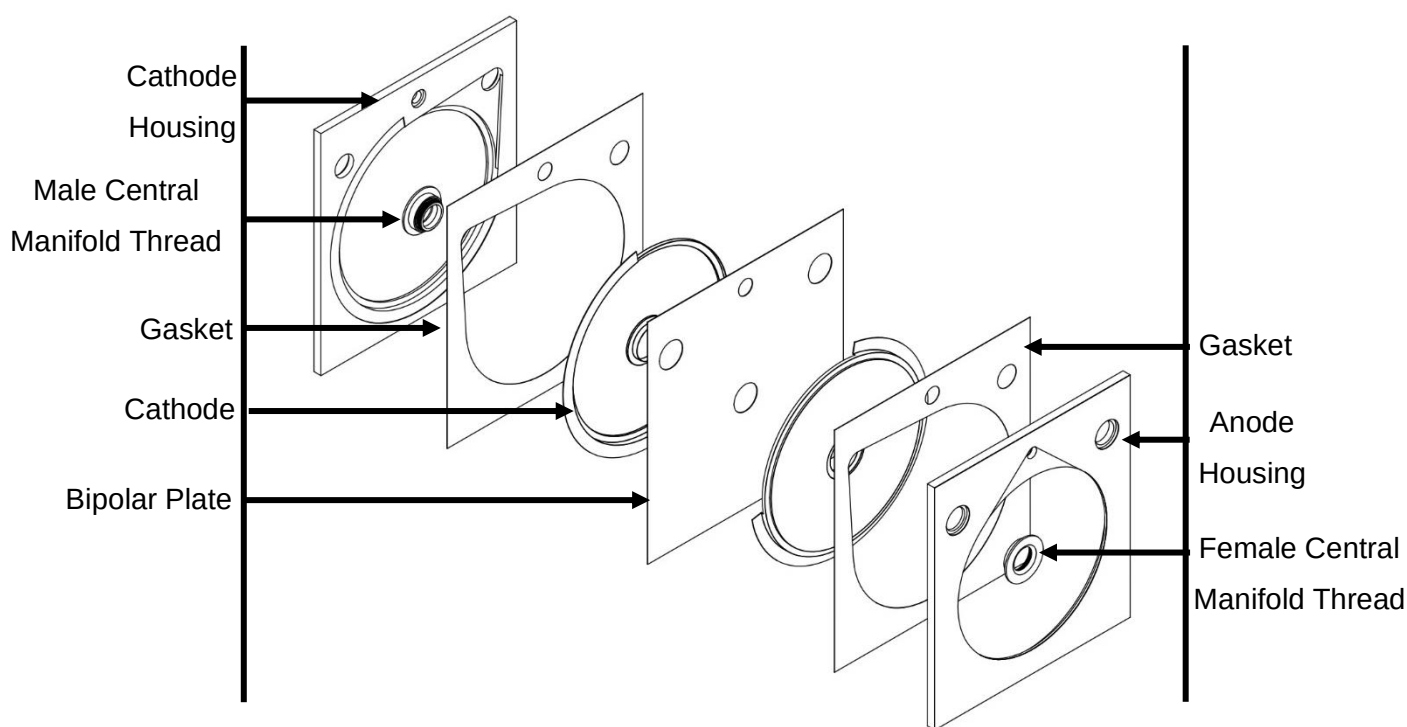


**Figure 5-4: Finalised scaled 320 cm electrode Bipolar Bi-MCFP design**

A total of 25 pairs were placed in series to produce a stack that is capable of producing 3 – 5 kg/day H<sub>2</sub> within the 2 – 2.4 VDC range. A schematic of the assembled stack is provided in Figure 5-5. With each electrode having an area of 754 cm<sup>2</sup>, the stack contains a total cathodic area of 1.885 m<sup>2</sup>, therefore, reaching a current density of 294 mA.cm<sup>2</sup> would result in 5 kg/day H<sub>2</sub> production.

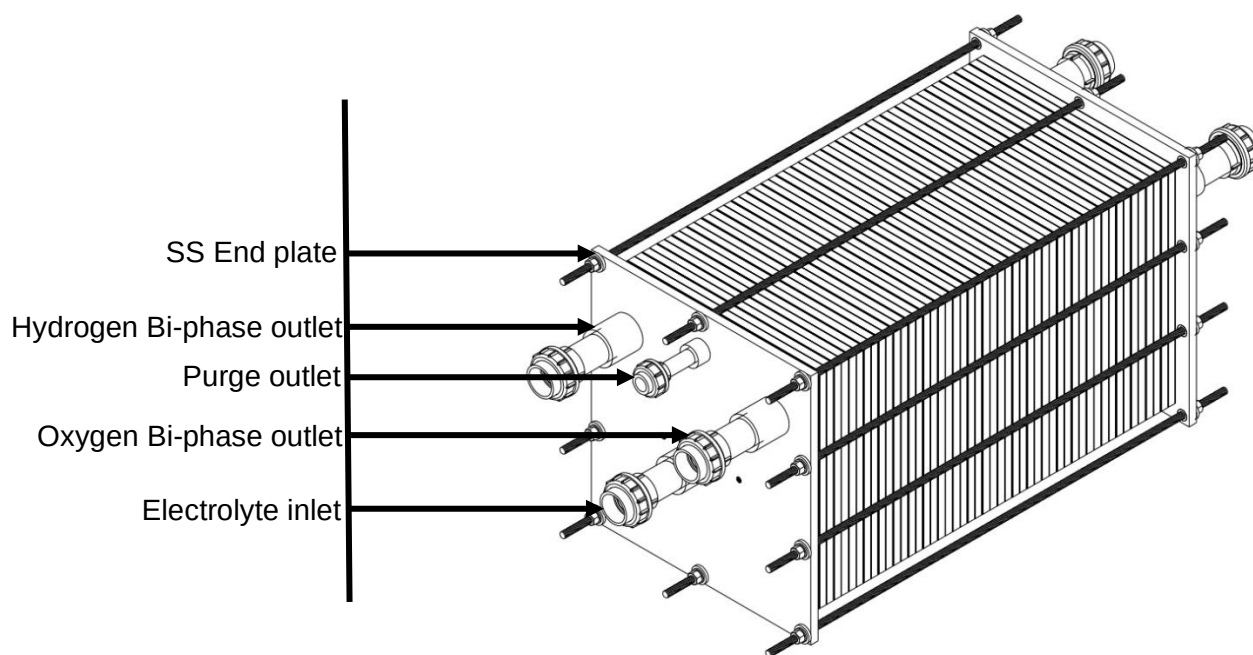


**Figure 5-5: 25 cell Bipolar Bi-MCFP stack containing 320 mm annular electrodes**

### 5.3.2 Balance of Plant

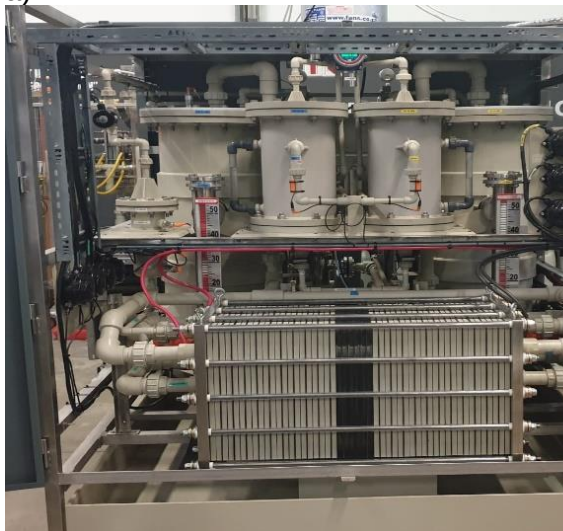
The following is a brief operational description of the pilot plant based on the attached P&ID diagram (see Appendix C):

- 1.1.1. The desired hydrogen gas is generated using electrolysis, which occurs within the alkaline water electrolyser (01-R-001).
- 1.1.2. DC power is fed to the electrolyser employing a switch-mode power supply (001-RF-002). The switch-mode power supply accepts 3 phase AC power as an input, and employing a rectifier, outputs variable DC power.
- 1.1.3. Purge gas generated within the electrolyser (01-R-001), is set to collect (through natural buoyancy) in a purge vessel (01-PR-015). The liquid level, and hence, dispensing of the purge gas from the vessel, is managed using a control valve and level sensors.
- 1.1.4. The purge gas is vented to the atmosphere.

- 1.1.5. Electrolytic solution (potassium hydroxide) is circulated through the electrolyser (01-R-001) using a circulation pump (01-P-005) under VSD (variable speed drive) control.
- 1.1.6. Excess heat generated in the electrolyser is removed using an air-cooled fin and tube heat exchanger (01-HX-006). The heat exchanger surface is cooled using cool air supplied by a low power fan (01-FAN-010) installed into the heat exchanger's framework.
- 1.1.7. De-ionised water is generated employing a de-ionisation system consisting of a series of reverse osmosis (RO )membranes and ion-exchange resin canisters (04-RO-017). Mains water is fed to the de-ionisation system by either mains pressure or a mains water pump providing the necessary pressure driving force to pass water through the de-ionisation system for collection in the de-ionised water holding tank (04-TK-016).
- 1.1.8. From the electrolyser (01-R-001), two bi-phase solutions result (electrolytic solution saturated with hydrogen and oxygen). The oxygen bi-phase solution enters a gas-lye separation vessel (01-S-003) and the hydrogen bi-phase enters a separate gas-lye separation vessel (01-S-004).
- 1.1.9. The separated lye from each vessel is re-combined where it is recycled through the heat exchanger (01-HX-006) to the electrolyte circulation pump (01-P-005).
- 1.1.10. Water is consumed within the electrolysis process, which results in reducing the liquid level within the gas-lye separation vessels. The level of the electrolytic solution is maintained in the gas-lye separation vessels using a de-ionised water dosing pump (04-P-009) which is fed with de-ionised water, from the de-ionised water holding tank (04-TK-016), into oxygen and hydrogen gas scrubbers (03-W-007 and 02-W-008).
- 1.1.11. Dosing the gas scrubbers with de-ionised water maintains a solution with a low potassium hydroxide concentration within the vessel, hence, the oxygen or hydrogen gas, separated in the gas-lye separators, is passed through this solution that works to remove any residual KOH carried over from the gas-lye separators. The gas scrubbers incorporate a liquid overflow allowing for the free-flow of liquid to the gas-lye separators.
- 1.1.12. The oxygen and hydrogen gas outputs from the gas scrubbers (03-W-007 and 02-W-008) are then passed through individual moisture traps (03-T-011 and 02-T-012) to remove any residual water carried over from the gas scrubbers. The fluid that accumulates within the water traps will be dispensed periodically under the action of a capacitance sensor and solenoid valves (SV009 and SV010).
- 1.1.13. The purity of the respective oxygen and hydrogen gas streams is monitored through online gas purity monitors (02-PM-013 and 02-PM-014).
- 1.1.14. Flashback arrestors (FA001 and FA002) are installed at the respective oxygen and hydrogen discharge points as a safety precaution.
- 1.1.15. Within the system enclosure, the surrounding gases will be analysed for flammable gas accumulation using a gas detector (01-PM-018).

Images of the pilot plant are provided in Figure 5-6. It is important to note that stack power consumption, pump power consumption and overall power consumption are monitored with the use of 3 power meters (green power meters depicted in Figure 5-6f), which provided realistic consumption values that are utilised in this study.

a)



b)



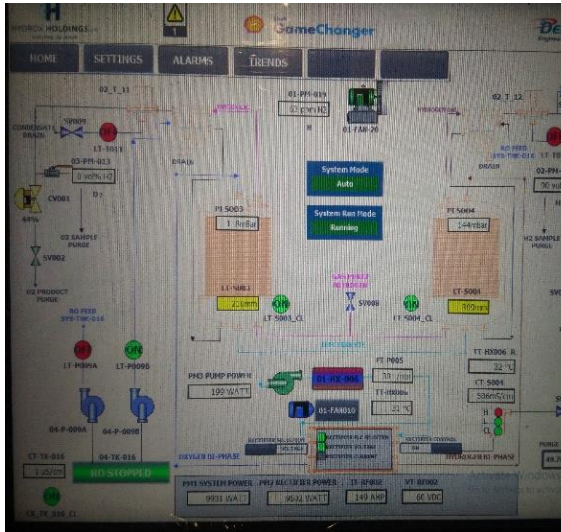
c)



d)



e)



f)



g)



h)



**Figure 5-6:** Images of the a) Electrolyser stack and BOP of DEFT™ 2.5 unit, b) scrubber units for product gases, c) gravitational separator, d) back of DEFT™ 2.5 plant - sampling panels, condensate drain, magnetic strainer and heat exchanger, e) Scada screen, f) internal of electrical panel, g) external of control panel and rectifier, and h) electrolyser stack.

### 5.3.3 Experimental Procedure

To evaluate the performance of the 5 kg/day H<sub>2</sub> Bipolar Bi-MCFP technology, the following tests were conducted to obtain performance indicators for the unit:

- a) start-up polarisation tests
- b) gas quality at different operating temperatures, and
- c) confirmation polarisation tests.

The objectives of the above-mentioned tests were to determine the effect and improvement associated with the reduced electrolytic flow on the performance of and the quality of gas produced from an electrolyser operating off the DEFT™ principle. As such, electrolytic flowrates at different operating temperatures were key variables in the above-mentioned tests. From this data, the performance and associated economics of the DEFT™ technology could be compared to industrial benchmarks to assess the technology's economic viability in the electrolytic hydrogen production market.

For testing, plain dutch weave of micron rating 80 µm and alloy nickel 200 was used as a basis for all investigations, and the electrolytic stack was in the form of a scaled Bipolar Bi-MCFP configuration, with the double-ended bi-phase collection and double injection through the centre of the stack, i.e. the configuration selection determined from observations in Section 4. With successful tests showing high purity (>99.5 vol% H<sub>2</sub>) gas production at a flow velocity of 0.0003 m.s<sup>-1</sup>, the goal was to operate the DEFT™ 2.5 pilot plant at even lower flow velocities (0.0002 m.s<sup>-1</sup> and lower). For this investigation, the DEFT™ 2.5 electrolysis stack was set up as follows:

- nickel mesh of a dutch weave configuration – no catalysts were employed,
- electrodes were etched in HCl to enhance the active surface area,
- pure nickel bi-polar plates to act as current carriers,
- Monofilament nylon 6 mesh (5 µm) was used as a non-conductive, hydro-dynamic layer. A micron rating of 5 µm was chosen,
- polypropylene housing plates and structural rings were employed,
- sealing gaskets were made from EPDM rubber to help seal the stack, and
- 30 wt% KOH electrolyte.

## 5.4 Results and Discussion

### 5.4.1 Start-up Polarisation Test

Polarisation tests were conducted at three different operating temperatures, namely 40°C, 60°C and 80°C, with three tests having been carried out for each operating temperature. Low, medium and high flows were tested at flow rates of 11.31, 22.62 and 45.24 L/min respectively while operating voltages were varied within a range of 1.8 – 2.4 VDC for each flow rate. From this, three performance indicators were derived, namely:

- IV data and subsequent system efficiencies,
- energy consumption data, and
- product gas purities.

Each of these performance indicators were evaluated at the above-mentioned temperatures and flow rates (Figure 5-7).

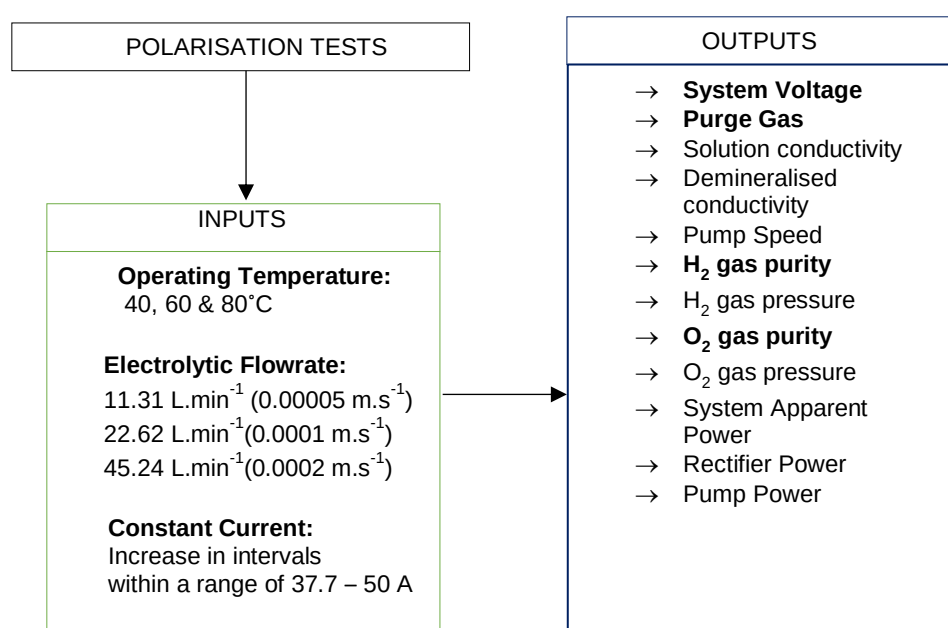


**Figure 5-7: Breakdown of variables for polarisation tests for the DEFT™ 2.5 system**

### 5.4.1.1 IV and System Efficiencies

In this section IV and power consumption data points are provided in Figure 5-8, Figure 5-9, and Figure 5-10. The discussion surrounding the IV data and power consumption follows within Section 5.4.1.2 and Section 5.4.1.3 respectively.

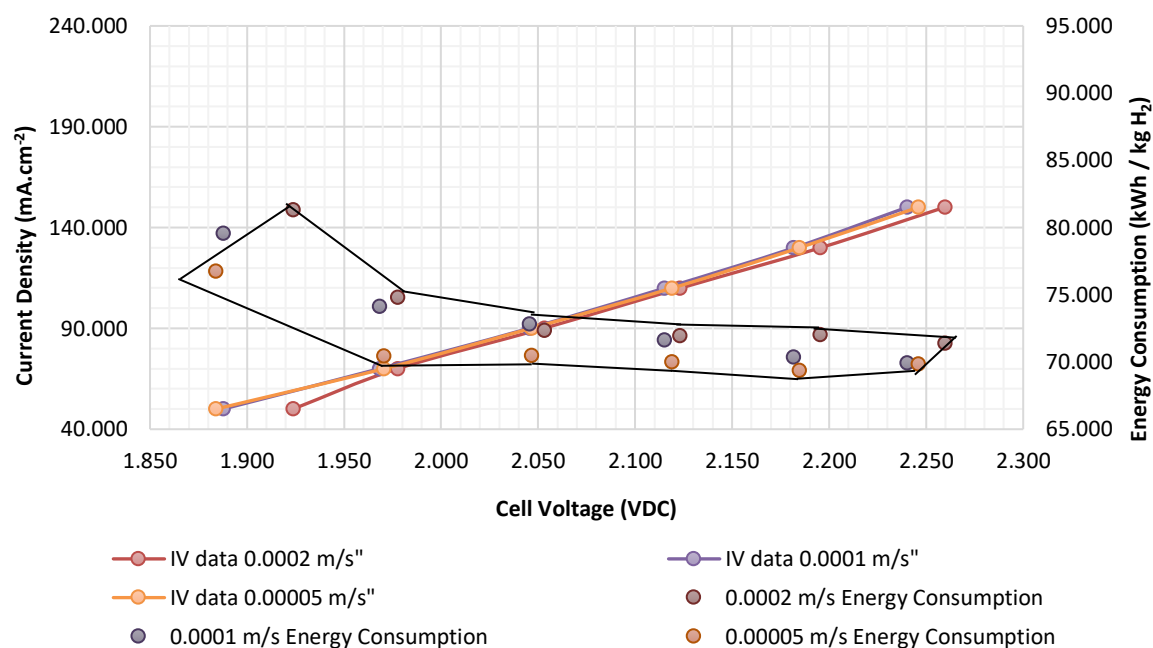


**Figure 5-8: IV and energy data for 40°C at various flow velocities for the DEFT™ 2.5 system**

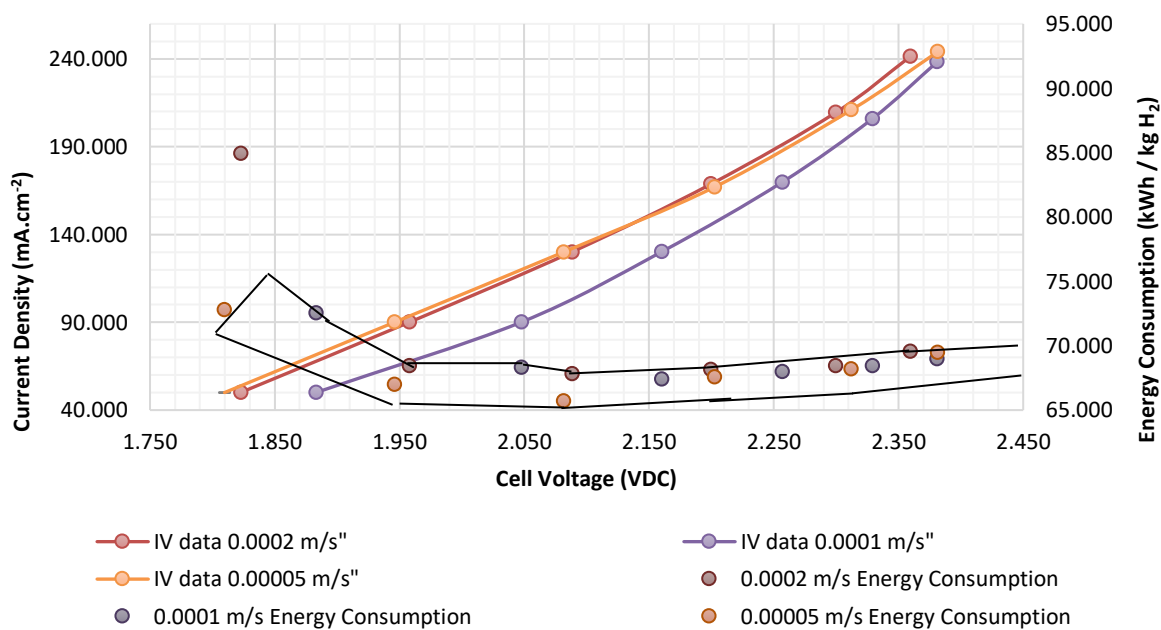


**Figure 5-9: IV and energy data for 60°C at various flow velocities for the DEFT™ 2.5 system**

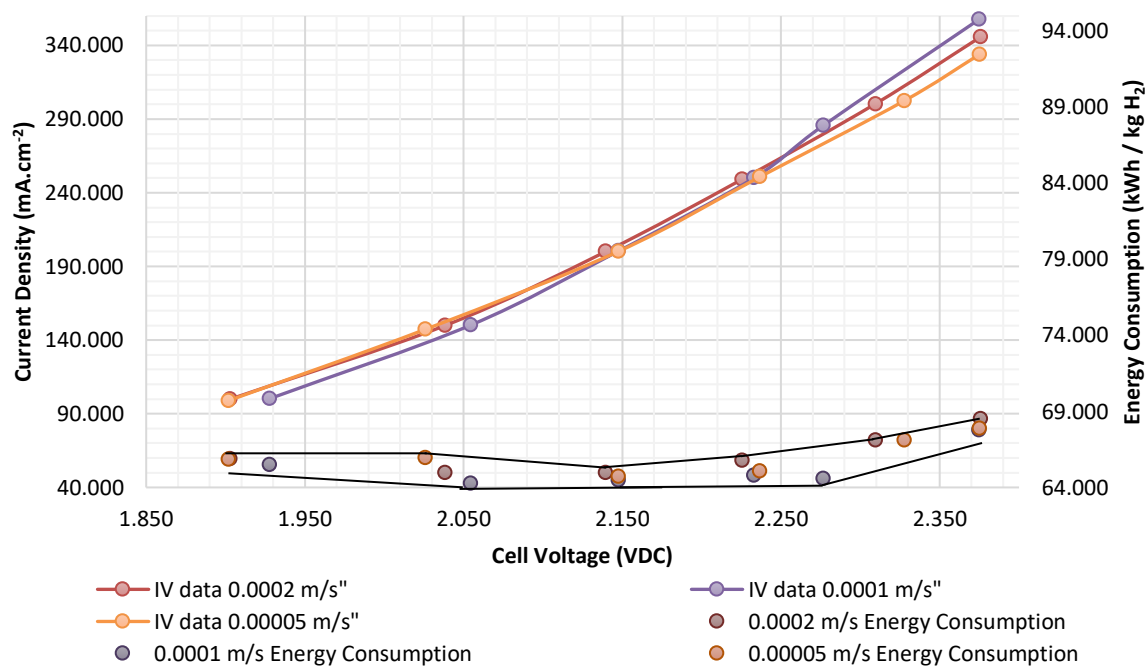


**Figure 5-10: IV and energy data for 80°C at various flow velocities for the DEFT™ 2.5 system**

#### 5.4.1.2 IV Data Analysis

The DEFT™ 2.5 system was able to achieve current densities between 90 to 345 mA.cm<sup>-2</sup> at 80°C, within the voltage range of 1.8 to 2.4 VDC. The expected improvement in current densities with temperature was observed for the DEFT™ system. Table 5-1 shows the effect of temperature and electrolytic flowrate on current density:

**Table 5-1: Improvement of current density (mA.cm<sup>-2</sup>) with varied electrolytic flow (L.min<sup>-1</sup>) and temperature (°C)**

| Temperature<br>(°C)  | 0.0002 m.s <sup>-1</sup> | 0.0001 m.s <sup>-1</sup> | 0.00005 m.s <sup>-1</sup> |
|----------------------|--------------------------|--------------------------|---------------------------|
| 80 (2.38 ± 0.01 VDC) | 345 ± 1.4                | 357.0 ± 1.3              | 333 ± 1.7                 |
| 60 (2.38 ± 0.01 VDC) | 241 ± 4.8                | 238 ± 4.4                | 244 ± 2.0                 |
| 40 (2.20 ± 0.01 VDC) | 150 ± 0.08               | 150.0 ± 0.1              | 150.0 ± 0.04              |

\*Percentage change in current density with temperature

\* Percentage change in current density with flow

The current density figures indicated in Table 5-1 are the maximum values achieved during the respective test runs. The blue and red values refer to improvements with increasing temperature and decreasing flow respectively. It is noted that flow velocity has little effect on current density, with little to no improvement observed at both low and high operating voltages. For a flow-through system, it can be expected that operating at higher flows will result in higher current densities due to the reduction in bubble coverage and subsequently, the ohmic resistance of the cell, however, at the low-end velocity range increases in flow velocity has little effect on cell performance. This behaviour can be observed at 80°C where the current density is observed to be the highest and therefore it is expected to exhibit the greatest improvement with increasing flow. The reduction in flow from 0.0002 to 0.0001 m.s<sup>-1</sup> resulted in an increase in current density (3.5% increase), however, further reduction in flow from 0.0001 to 0.00005 m.s<sup>-1</sup> resulted in a decrease in current density (6.7% decrease). The percentage change is, however, insignificant falling within the range of irreproducibility expectations due to the existence of random errors. It is apparent that at the low-velocity ranges flow optimisation for performance (targeting increased current density via flow increases) is not warranted. The primary objective would therefore be to minimise the flow velocity such that it allows for adequate gas separation, therefore, minimising parasitic loads.

The current density data provided in Figure 5-9 and Figure 5-10 show similar current density performance when compared to IV data provided for the Bi-MCFP pilot at 0.001 m.s<sup>-1</sup> (Figure 3-13), therefore, no indication of performance degradation has been noted with the incorporation of bipolar plates or with scale-up and further reductions in flow.

The data points for 0.0001 m.s<sup>-1</sup> and 60°C shows a significant decrease relative to the data obtained for flow velocity's 0.0002 and 0.00005 m.s<sup>-1</sup>. After checking the data historian it was noted that this result was the consequence of a drop in operating temperature, due to a slow response/error in the PID control system with the low current densities not being reflective of the flowrate, but rather of a drop in temperature. The data obtained and provided in Figure 5-8, Figure 5-9 and Figure 5-10, will form the basis of several assessments in the following sections of this dissertation.

### 5.4.1.3 Overall System Energy Consumption Analysis

**Table 5-2: Energy, IV and Production rate data for the DEFT™ 2.5 unit - 80°C**

| Flow<br>(L/min) | Energy Consumption<br>(kWh/kg) | Production Rate<br>(kg/day H <sub>2</sub> ) | Current Density<br>(mA.cm <sup>-2</sup> ) | Voltage<br>(VDC) |
|-----------------|--------------------------------|---------------------------------------------|-------------------------------------------|------------------|
| H               | 65.105                         | 3.469                                       | 203.8 ± 0.35                              | 2.15 ± 0.01      |
| M               | 64.462                         | 3.409                                       | 200.4 ± 0.19                              | 2.15 ± 0.01      |
| L               | 64.696                         | 3.405                                       | 200.1 ± 0.23                              | 2.15 ± 0.01      |

The lowest energy consumption points for the DEFT™ 2.5 system were achieved at 80°C. Higher flows resulted in slightly better current densities and production rates, in comparison to the medium and lower flow rates, at the expense of higher energy consumption. Improvements in the energy consumption of the system were observed with decreased parasitic loads, however, at 80°C, operation at a low electrolytic flow resulted in slightly higher energy consumptions in comparison to medium flows. This is because a higher current density was noted at 0.00005 m.s<sup>-1</sup> compared to 0.0001 m.s<sup>-1</sup>, however, as noted previously, this difference is within the margin of error, therefore, with fairly similar current densities slight improvements in overall efficiency can be expected with lower flowrates (reduced parasitic loads).

At an operating temperature of 80°C, reducing the flowrate from 45.24 L.min<sup>-1</sup> (0.0002 m.s<sup>-1</sup>) to 22.5 L.min<sup>-1</sup> (0.0001 m.s<sup>-1</sup>), an improvement of 0.99% in overall power consumption is associated with a 1.73%, and 1.6% reduction in production rate and current density respectively. These improvements/reductions are, however, negligible, thus indicating that the parasitic load no longer carries a large weighting in the determination of the overall power consumption of the system. The weighting of such will be analysed within the following sections. It is, however worth noting that system efficiencies before the commencement of this study, as reported by Gillespie *et al.*, equated to 12 – 16 HHV% (328.33 – 246.25 kWh/kg H<sub>2</sub>) with maximum values just below 35 HHV% achieved at over 3 VDC [1], [22]. Within the 2.1 – 2.2 VDC range, this translate to 3.8 – 5.2 times reduction in power consumption while experiencing roughly a 2 – 2.5 times reduction in current density. While there is indeed a reduction in ohmic losses observed at high electrolytic flow rates, the associated parasitic losses result in undesirable energy consumption. When the optimum balance between parasitic load and stack load is found, the improvements in performance associated with the increased flows are minimal to negligible.

Figure 5-8, Figure 5-9 and Figure 5-10 show the energy consumptions for the system within enclosed black regions. It can be observed that the width of these regions is larger at lower current densities and smaller at higher current densities. This indicates that the effect of parasitic load on

the overall energy consumption is greater at lower operating voltages, therefore, from an energy efficiency viewpoint, it is more beneficial to operate at lower flow rates when operating at partial loads. It can be observed, however, that at 80°C, the effect of the parasitic load on the system's overall energy consumption is lowered, due to larger stack loads, therefore, slightly higher flows may be employed to provide sufficient gas separation with little cost to the overall system efficiencies.

#### 5.4.1.4 Energy Data at Varied Temperatures and Flowrates

In this section energy and production capacity data points are provided in Figure 5-11, Figure 5-12, and Figure 5-13. The discussion surrounding the energy and hydrogen production capacity data follows within Section 5.4.1.5 and Section 5.4.1.6 respectively.

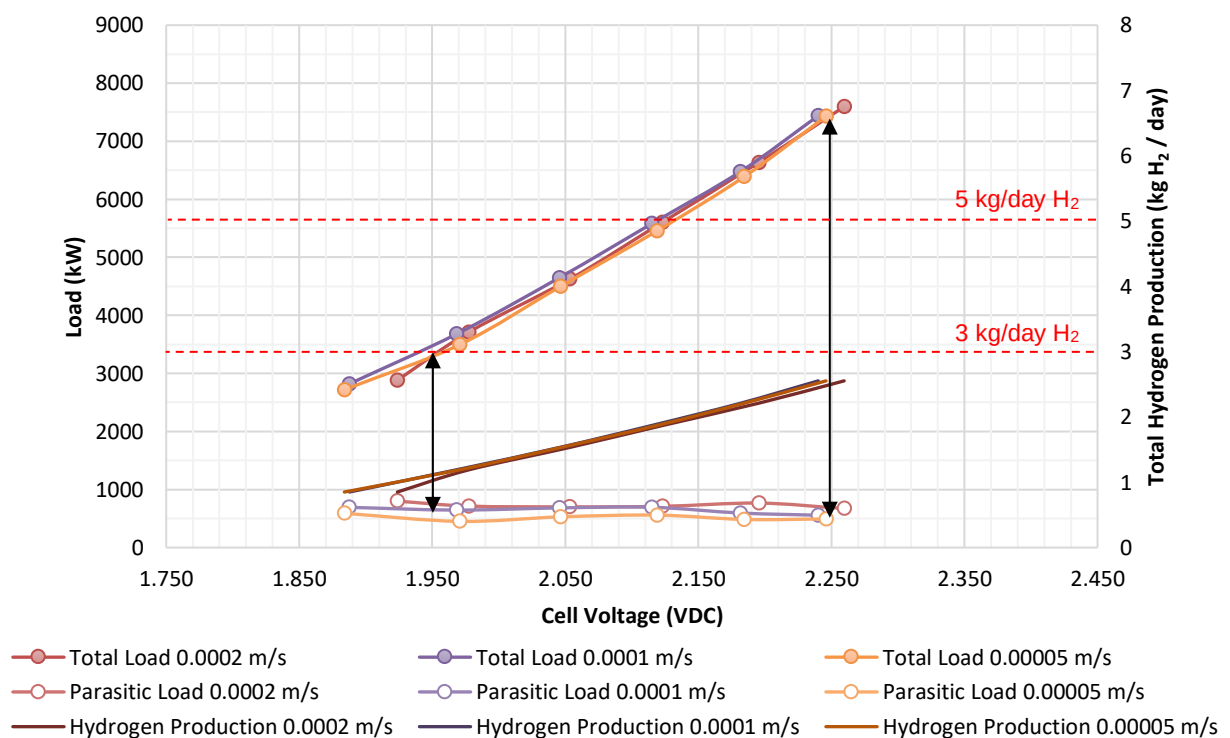


**Figure 5-11: Energy Data (kW) for DEFT™ 2.5 unit at varied flow rates and 40°C**

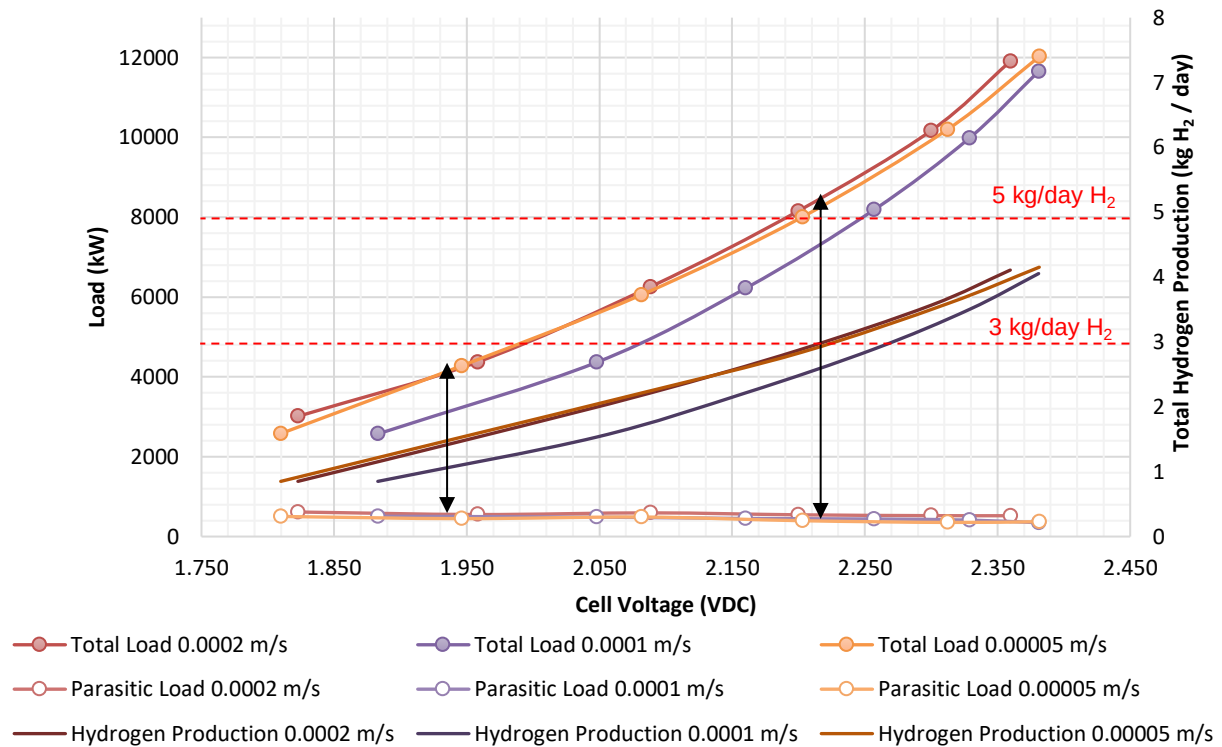


**Figure 5-12: Energy Data (kW) for DEFT™ 2.5 unit at varied flow rates and 60°C**

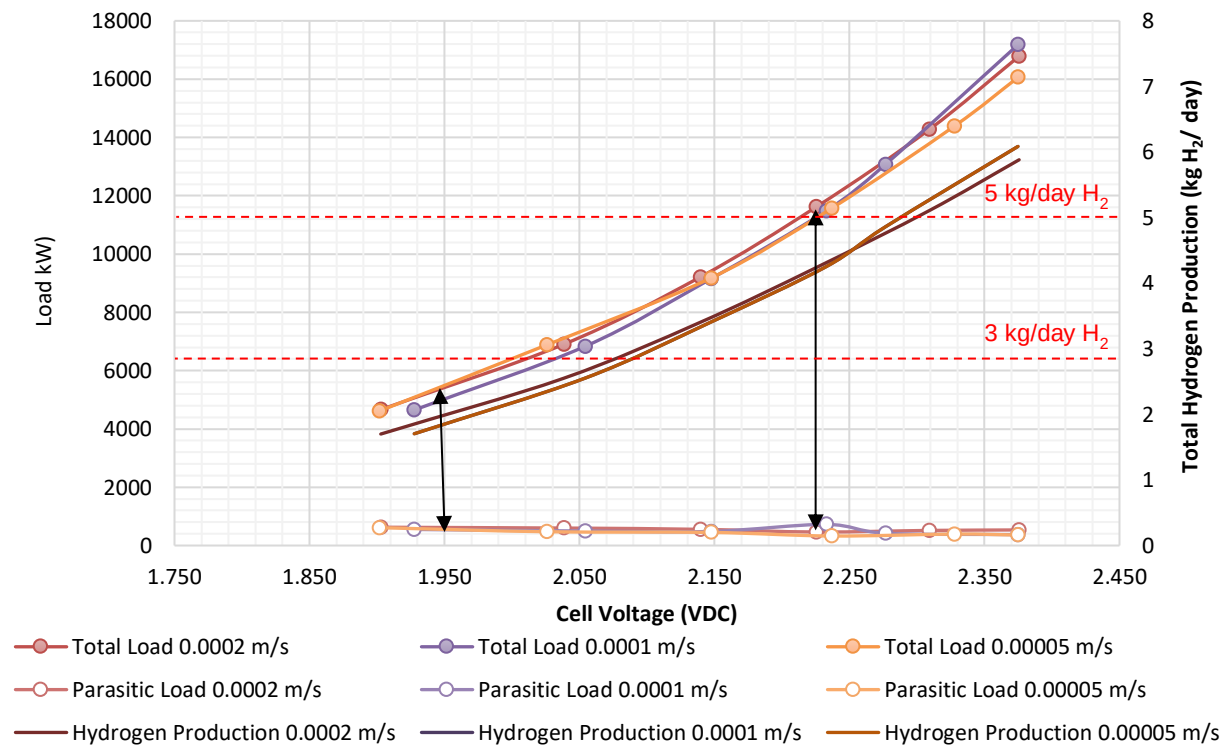


**Figure 5-13: Energy Data (kW) for DEFT™ 2.5 unit at varied flow rates and 80°C**

#### 5.4.1.5 Analysis of Energy Consumption Data at Varied Temperatures and Flowrates

Figure 5-11, Figure 5-12 and Figure 5-13 show similar trends to that of the IV and energy consumption data for the DEFT™ 2.5 unit. The load capacity of the unit increases with temperature, as expected, due to the added benefits of heat ( $T\Delta S$ ). Varied flowrates resulted in similar load capacities with very little deviation being observed between curves. The most significant deviations observed for the system load curves can be seen at lower operating voltages and hence, lower current densities. The parasitic load for the system varied between 627 - 359 W across the range of operating voltages.

**Table 5-3: Parasitic load and pump load weighting towards overall power consumption for the DEFT™ 2.5 unit - 80°C, 0.0002 m.s<sup>-1</sup>**

| Voltage (VDC) | Stack Power (W) | Rectifier Eff | Parasitic Power (W) | Pump Power (W) | System Power (W) | %Pump Load | %Parasitic Load |
|---------------|-----------------|---------------|---------------------|----------------|------------------|------------|-----------------|
| 1.90 ± 0.01   | 3 582           | 88.76%        | 627                 | 349            | 4 664            | 7.5%       | 13.5%           |
| 2.04 ± 0.01   | 5 758           | 91.36%        | 599                 | 337            | 6 902            | 4.9%       | 8.7%            |
| 2.14 ± 0.01   | 8 066           | 93.21%        | 556                 | 344            | 9 209            | 3.7%       | 6.0%            |
| 2.23 ± 0.01   | 10 453          | 93.70%        | 46                  | 339            | 11 620           | 2.9%       | 4.0%            |
| 2.31 ± 0.01   | 13 071          | 94.97%        | 518                 | 321            | 14 280           | 2.2%       | 3.6%            |
| 2.38 ± 0.01   | 15 482          | 95.24%        | 535                 | 314            | 16 789           | 1.9%       | 3.2%            |

The stack power consumption is determined through multiplying the stack voltage with the series current. As noted, the pump, rectifier and overall power consumption were measured and recorded. The rectifier efficiency was determined by the ratio of the stack voltage determined (IV multiplication) and the measured value. At 80°C and 0.0002 m.s<sup>-1</sup>, the pump accounts for 1.9 to 7.5 % of the plant's overall power consumption. This is a drastic improvement over the figures reported in Section 1.3.2. Generally, lower flowrates result in the lowest parasitic loads, with this being more observable at higher current densities and higher temperatures. An increase in temperature resulted in an overall drop in parasitic load. This is a result of the decreased viscosity of the electrolyte associated with higher temperature operation, as well as a decrease in fluid density and head requirement due to increased bubble production at higher current densities. Both of these factors contribute to a net lower parasitic load. This could be a result of the natural buoyancy and movement of gases formed within the electrolytic stack, which promotes flow through the product outlets thus reducing the pumping demand. Furthermore, increased current densities in the system also resulted in reduced parasitic load weightings, i.e. lower parasitic load contributions to kWh/kg H<sub>2</sub>. As observed in the IV and energy consumption data, at 40°C, the

contribution of the parasitic load towards the total system load ranged from 22% - 7%, with the upper bound at an operating voltage of ~1.9 VDC and the lower bound at ~2.4 VDC. Similarly, the parasitic load contribution for 60°C and 80°C are 19% - 3% and 13% - 2% respectively.

#### **5.4.1.6 Hydrogen Production Data**

The production rate requirements for the DEFT 2.5<sup>TM</sup> unit was set at between 3 - 5 kg/day H<sub>2</sub>. This size scale was selected as it provides a realistic view of an electrolyser unit operating at scale from which realistic economic and performance data could be obtained i.e. a small-scale commercial demonstration. The DEFT 2.5<sup>TM</sup> unit was able to achieve this at operating temperatures above 60°C. Below 60°C within the stipulated voltage range, the unit was only able to reach production rates of ~ 2.6 kg/day, which is just below the targeted rate. Production rates of the DEFT<sup>TM</sup> 2.5<sup>TM</sup> system were, however, improved with increased operating temperatures. Increasing the temperature from 40-60°C and from 60-80°C, improvements of 42% and 28% were observed, respectively. At 60°C, the targeted production rate was only achieved at higher operating voltages, which is indicative of low system and stack efficiency which is undesirable. At 80°C, however, the system was able to produce the stipulated production rate within reasonable system efficiencies achieving the 3 kg/day H<sub>2</sub> production target at ~2 VDC and the 5 kg/day H<sub>2</sub> production target at ~2.2 VDC. The system, however, was unoptimised during this testing phase. With the employment of an appropriate catalyst and the improvement of the electrode assembly, higher production rates can be achieved at lower voltages/higher efficiencies.

As already noted, the observable effect of electrolytic flow rate on hydrogen production is negligible at the low-velocity range. Small deviations between the flowrate curves can be observed at lower and higher current densities. The flow rate-production curves follow the same trend as the IV curves as the current density of the system determines the production rate of hydrogen.

At 60°C, a large deviation of the medium flow curve is observed, which is a result of the notable temperature drop of the system. It is further observed that high electrolytic flow at low current densities results in slightly higher production rates in comparison to low flows. At 80°C, operating at high flows results in only a 5% improvement of the production rate, in comparison to low electrolytic flows, and does not warrant the high costs associated with high parasitic loads.

### 5.4.1.7 Gas Purities at Varied Temperature and Flowrates

In this section hydrogen and oxygen gas purity data is provided in Figure 5-14, Figure 5-15, and Figure 5-16. The discussion surrounding the hydrogen and oxygen gas purity data follows within Section 5.4.1.8.

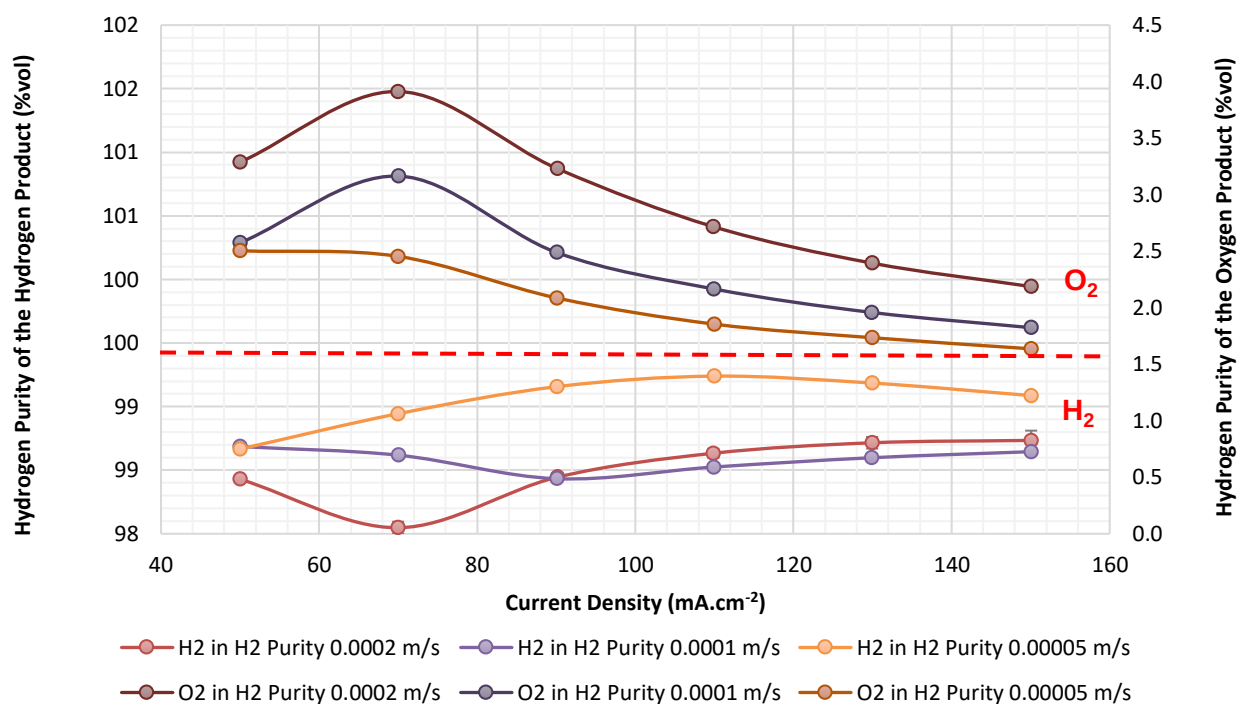


Figure 5-14: Gas Purity Data (vol%) for DEFT™ 2.5 unit at varied flow rates and 40°C

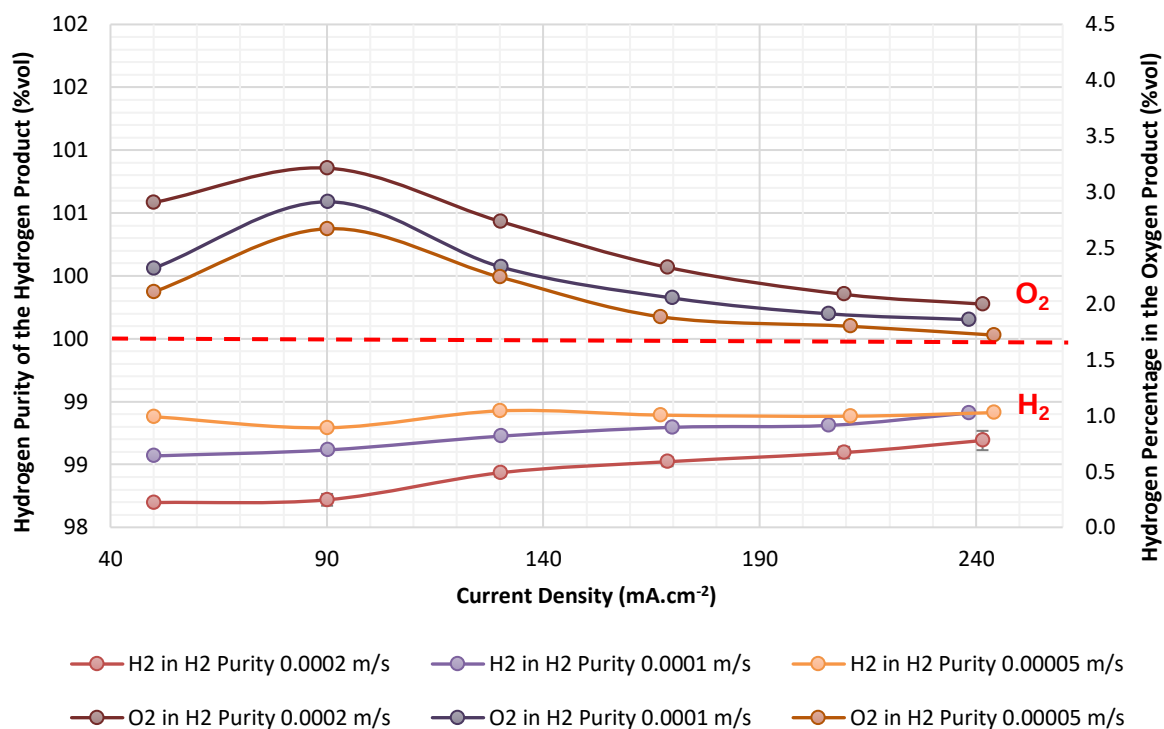


Figure 5-15: Gas Purity Data (vol%) for DEFT™ 2.5 unit at varied flow rates and 60°C

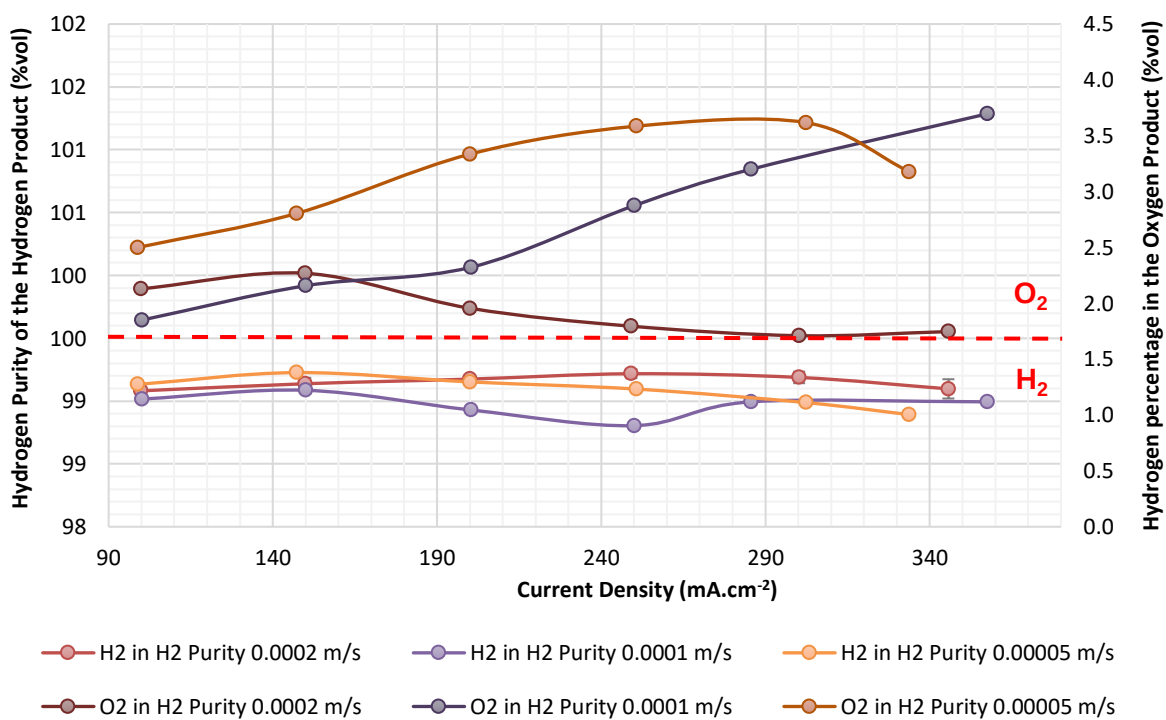


Figure 5-16: Gas Purity Data (vol%) for DEFT™ 2.5 unit at varied flow rates and 80°C

#### 5.4.1.8 Hydrogen and Oxygen Gas Purity Analysis

The flammability range for hydrogen in oxygen is between 94 – 4 vol% [104]. To safely operate electrolysis systems, industrial norms allow for product purities to reach 50% of the flammability range before a system shut down occurs, therefore, a hydrogen purity of > 97 vol% and < 2 vol% must be maintained during production. For the DEFT™ 2.5 unit, a hydrogen product purity of > 99.5 vol% was targeted. The objective of these tests was to determine whether a flow-through system, in the configuration of the DEFT™ 2.5 unit, would be capable of providing adequate product gas separation at the reduced flow velocities.

In reference to Figure 5-14, Figure 5-15, and Figure 5-16, the DEFT™ 2.5 unit was able to achieve hydrogen purities between 98 – 99.2 vol% across the flow velocity ranges, with the best hydrogen purities being achieved at higher temperatures. The DEFT™ system was not able to achieve a continuous steady-state hydrogen purity of > 99.5 vol%, however, this purity point (and greater) can be achieved with the employment of additional purification units. The DEFT™ 2.5 system was, however, able to achieve hydrogen purities that are within the realms of the safe operating range for electrolysis systems. The inability to meet the continuous steady-state hydrogen purity of > 99.5 vol% could be due to ineffective separation in the electrolyser stack or due to recirculation of product gases from the gas-lye separators (deviations from 100% separation efficiency). Little to no trends are observed in the hydrogen gas purity with changing current density and temperature besides a slight drop off in hydrogen gas purity at greater current densities (noted in Figure 5-16 at > 240 mA.cm<sup>-2</sup>). The change in purity is insignificant, however, the trend is observable.

The flammability limit for hydrogen in oxygen is ~ 4 vol% [104]. At 40°C, Figure 5-14, the oxygen purity came close to the flammability limit when operating at low current densities but improved significantly when current densities were increased. An increase in temperature to 60°C resulted in an improvement in the oxygen purities, as per Figure 5-15. High current densities and lower flowrates, therefore, resulted in improved oxygen purities between the temperatures of 40 - 60°C. At 80°C, Figure 5-16, the oxygen purity became erratic, with impurities approaching the explosive limits when operating at low and medium flows. This phenomenon was further investigated during the gas quality degradation tests, Section 5.4.2, where the cause of the observed problem (equipment error) was investigated. In addition to an equipment error, the poor oxygen qualities at 80 °C could be a result of thermal changes to the nylon separator material, as 80 °C is greater than the glass-transition temperature of nylon [105]. As such, the cross-gas contamination was heightened in the system causing significant contamination of the oxygen product (this effect, however, was not noted on the hydrogen side). Consequently, greater electrolytic flows were

required to achieve adequate separation, and this was observed in the purity data. The decrease in oxygen purity with increasing flowrates (noted in Figure 5-14 and Figure 5-15) and decreasing temperatures is also symptomatic of inefficiencies in gas-lye separation. As previously tested, gas separation improves with increasing flow velocities, as noted in Table 1-1 and Figure 3-12. Increasing flow velocities, however, result in increased gas re-entrapment as well as reduced bubble coalition (reduced buoyancy forces), and hence some inefficiencies in gas-lye separation are predicted. Secondly, gas-lye separation efficiencies improve with temperature thus explaining the decrease in oxygen gas purity with decreasing temperature.

It is reported in literature that hydrogen has a higher gas diffusion coefficient compared to oxygen (estimated to be 6 times greater at 60°C) and hence lower oxygen product purities are normally observed compared to that of hydrogen product purities [106]. This high gas diffusion coefficient is the cause for inadequate operation exhibited by liquid alkaline electrolyzers at low current densities. Higher current densities work to reduce the concentration of the impurity gas (hydrogen) reference to the oxygen product through dilution. This phenomenon was expected and is noted in the trends of the oxygen gas purity curves presented in Figure 5-14, Figure 5-15 and Figure 5-16. It is believed that the reduced oxygen gas purity is as a consequence of a multitude of sources, however, the extent of the change in the oxygen purity, from low to high current densities, can be used as an indication as to what contribution inadequate gas separation in the electrolyser plays in this matter.

From Figure 5-14 Figure 5-15 and Figure 5-16 it is noted that all three flowrates were capable of maintaining hydrogen gas purities that were deemed within the safe operating range. Oxygen gas purities, however, were noted to be dependent on flow rate and current density with acceptable gas purities achieved at 140 mA.cm<sup>-2</sup> and higher.

#### **5.4.2 Gas Quality Degradation with Increased Stack Operation.**

Deteriorations in oxygen purities were observed at higher temperatures. Running tests at temperatures higher than 60°C became problematic, as purity safety interlocks were activated due to the low oxygen purities (high H<sub>2</sub> contaminate). The hydrogen and oxygen purities were observed at different periods during the stack's operation, to determine the temperatures and conditions at which the DEFT™ 2.5 system operated safely. Four tests were conducted at different points in the lifespan of the stack, to observe the effect of operating time on product gas purities.

**Table 5-4: Objectives of tests observing the degradation of gas purities with time.**

| Test | Objectives of the test                                                                                                                                                          |
|------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 1    | Observe gas purity trends from the DEFT™ 2.5 stack after an extended period of operation.                                                                                       |
| 2    | Re-assemble stack and remove electrolytic sludge from electrode assembly. Operate the stack to observe gas purities.                                                            |
| 3    | Determine the remedial actions required to restore gas purities to acceptable levels – the test will be conducted on the stack used in test 2.                                  |
| 4    | Determine the effect of an additional locking ring to the electrode assembly on gas purities – This test will be conducted on a reassembled stack with an additional component. |

#### **5.4.2.1 Gas Purity Degradation Test 1 – Monitoring Gas Purity on an Operating Stack.**

During the 80°C test, noticeable deteriorations in gas purities were noticed, such that safety interlocks on the oxygen side of the plant were triggered, which prevented continuous stability tests from being carried out. The 80°C test showed reduced oxygen purities at similar gas current densities as noted for 40°C and 60°C. The 80°C start-up polarisation tests were the last of the polarisation tests to be carried out, hence, temperature or time-based changes may have affected the operation of the stack. A test was conducted to observe the gas purities of both the hydrogen and oxygen product while heating the plant to an operating temperature of 80°C. The following results were obtained.

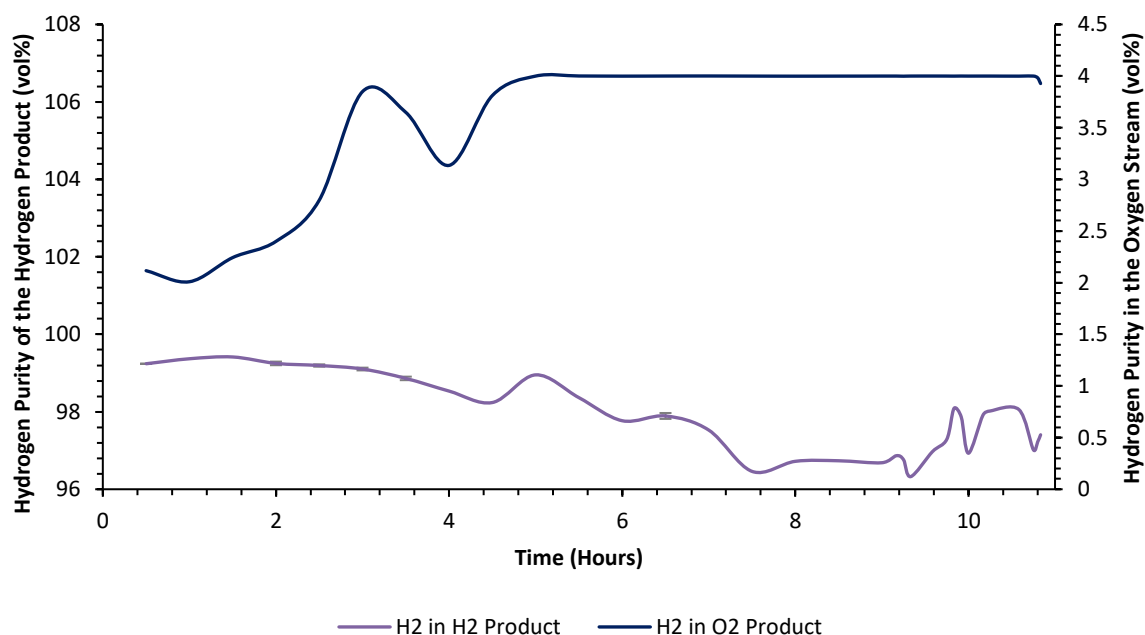


**Figure 5-17: Purity data (vol%) for Gas Purity degradation Test 1 for the DEFT™ 2.5 unit**

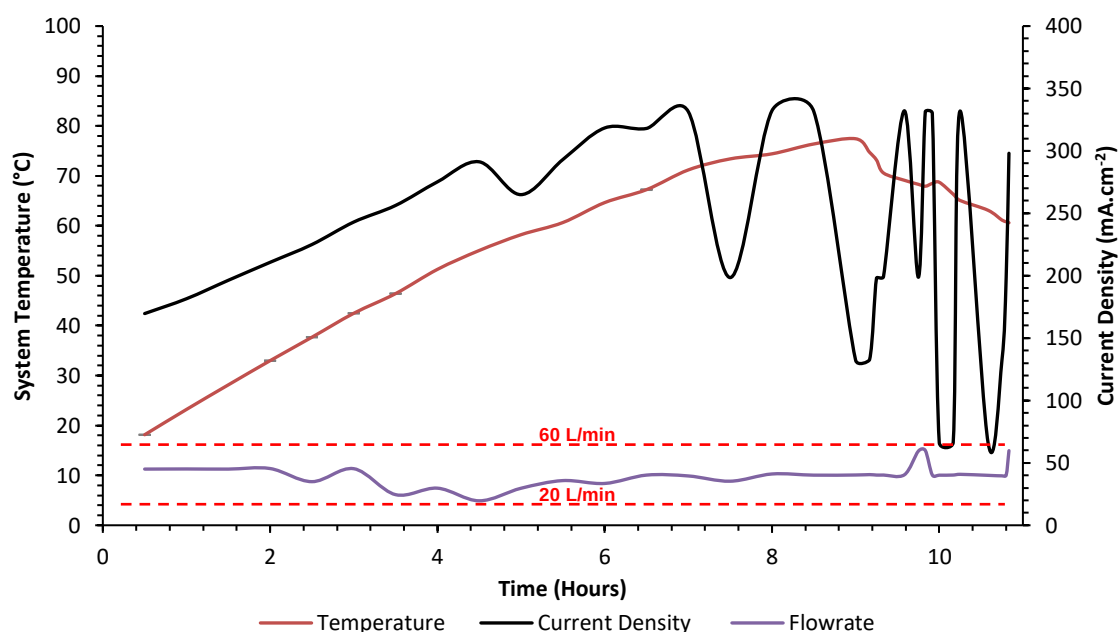


**Figure 5-18: Current density ( $\text{mA.cm}^{-2}$ ), operating temperature ( $^{\circ}\text{C}$ ) and electrolytic flowrate ( $\text{L.min}^{-1}$ ) data for Gas Purity degradation Test 1.**

Figure 5-17 and Figure 5-18 shows that the system was able to reach a max operating temperature of  $56^{\circ}\text{C}$  before the oxygen purities increased to  $\geq 4$  vol% hydrogen contamination, creating an explosive mixture. Figure 5-17 shows the oxygen gas purity levels maxed out at 4 vol%  $\text{H}_2$ , this is because the gas analyser installed on the oxygen product line has a 0 – 4 vol%  $\text{H}_2$  range. The electrolytic flowrate was maintained between 39 – 50  $\text{L/min}$  throughout the test. The current supply was varied at 8.6 hours into the test in an attempt to improve oxygen purities,

however, no improvement was noted, with the meter remaining at the maximum contamination of 4 vol%. The fluctuation in current density also caused hydrogen purities to drop close to the flammable limit between 7.8 – 8.8 hours into the test, as a result of the poor dilution of contaminants associated with lower current densities.

Data from the start-up polarisation tests show that the system was able to operate within the safe range of the flammable limit at 60°C. At 80°C, oxygen purities were flammable at lower and medium flowrates, but remained within the safe limits for high flowrates. In comparison, at the 60°C and high electrolytic flowrates, the DEFT™ stack, after a substantial operation duration, was not able to operate at safe gas purities. It was predicted that three possible changes to the stack could have caused the observed phenomena:

- 1) **The configuration of the electrode assembly changed with time or temperature** – It is possible that the electrodes moved or dislodged over time or due to expansion and contraction forces with temperature changes. This would significantly increase the cross-gas contamination within the system.
- 2) **Accumulation of electrolytic sludge on the non-conductive layer** – Electrolytic sludge was seen to build up over time in the liquid alkaline electrolyser due to contaminants found in the KOH solute or metals (Iron in particular) that have leached out of stainless steel components to later reduce as a powder on the cathode.
- 3) **The structural integrity of the nylon material used for the non-conductive layer has been compromised** – Deformation of the non-conductive layer will result in increased cross-gas contamination.

To identify the cause of the poor gas separation in the stack, three further tests were conducted on the DEFT™ stack.

#### **5.4.2.2 Gas Purity Degradation Test 2 – Removal of Electrolytic Sludge.**

Test 2 involved the opening of the electrolyser stack to remove the electrolytic sludge that accumulated within the stack. The constituents of the sludge were analysed through powder XRF (X-ray fluorescent) analyses. The composition of the sludge can be found in Appendix D. With the removal of volatiles and the exclusion of potassium, the sludge mainly comprised of nickel deposits (15.8%) with some iron noted (1.21%), with nickel expected to be within the electrolytic solution through dissociation of nickel components and iron through leaching of stainless steel components. The following results, Figure 5-19 and Figure 5-20, were obtained once the electrolytic sludge was removed.

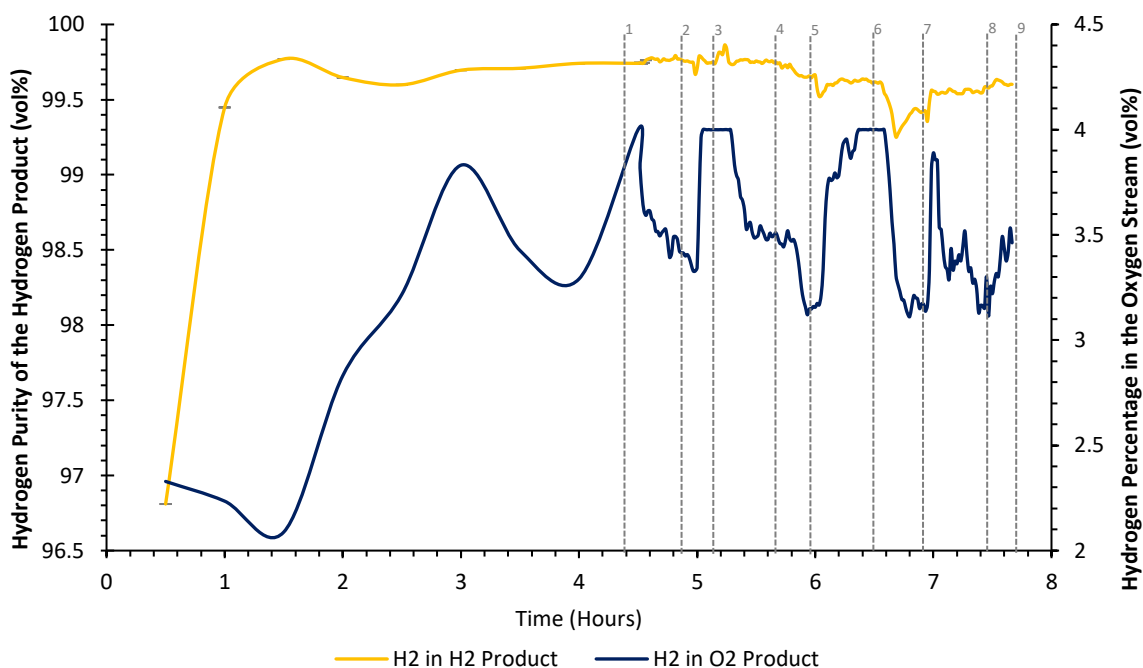


**Figure 5-19: Purity Data (vol%) for after the removal of the electrolytic sludge (Test 2)**

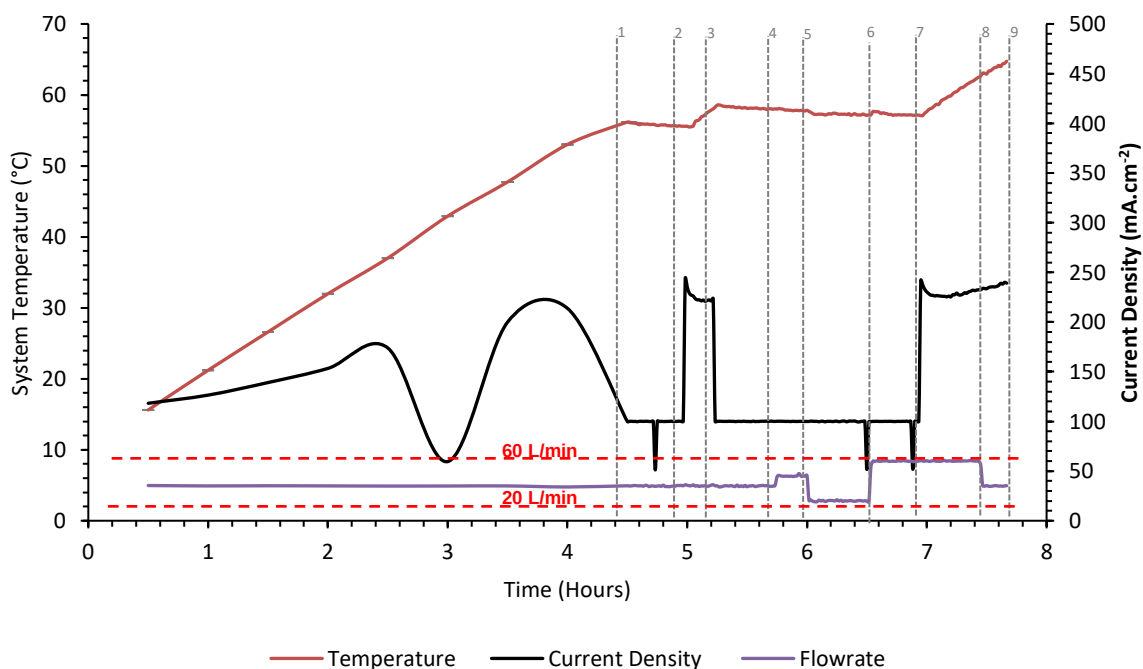


**Figure 5-20: Current density ( $\text{mA.cm}^{-2}$ ), operating temperature ( $^{\circ}\text{C}$ ) and electrolytic flowrate ( $\text{L.min}^{-1}$ ) data for the removal of electrolytic sludge (Test 2)**

With the removal of the electrolytic sludge, it was observed, as per Figure 5-19, that the re-assembled stack still produced oxygen purities  $\geq 4$  vol% hydrogen at temperatures  $\geq 56^{\circ}\text{C}$ . At 4.4 hours into the test, the current and electrolytic flow rate was varied to see the effect on the gas purities. It was observed that a drop in current density and an increase in electrolytic flow

rates (point 6 and 7) improved oxygen purities. It was found, however, that the oxygen purity began to decrease again after recovering. Furthermore, it was noted that recovering the oxygen gas purities became increasingly difficult as hydrogen contamination passed 4 vol%.

The removal of the electrolytic sludge ultimately did not have any observable effects on the product gas purities, and therefore the poor gas qualities observed is most likely due to a change in the position of the electrodes within the stack, or separator inefficiency.

### 5.4.2.3 Gas Purity Degradation Test 3 – Determining the Operating Range for Acceptable Gas Purities.

A third test was conducted to determine the effects of varying the operating conditions on gas purity and the possible operating range for the degraded stack. The conditions were varied in 10 different ways, and are listed in Table 5-5

**Table 5-5: Varied operating conditions for Gas Purity Degradation Test 3**

| Test No. | Description                                                                        |
|----------|------------------------------------------------------------------------------------|
| 1        | Increase flowrate to 45 L.min <sup>-1</sup>                                        |
| 2        | Decrease current to 200A.<br>Electrolytic flow increased to 60 L.min <sup>-1</sup> |
| 3        | Current increased to 250 A                                                         |
| 4        | Current dropped to 200 A                                                           |
| 5        | Current dropped to 150 A                                                           |
| 6        | Electrolytic flow to 45 L.min <sup>-1</sup>                                        |
| 7        | Current increased to 250 A                                                         |
| 8        | Current dropped to 200 A                                                           |
| 9        | Current dropped to 150 A                                                           |
| 10       | Electrolytic flowrate dropped to 20 L.min <sup>-1</sup> .                          |

Intentional changes in the operating conditions of the system are highlighted in grey in Table 5-5, while remedial actions to restore oxygen purities are left in white.

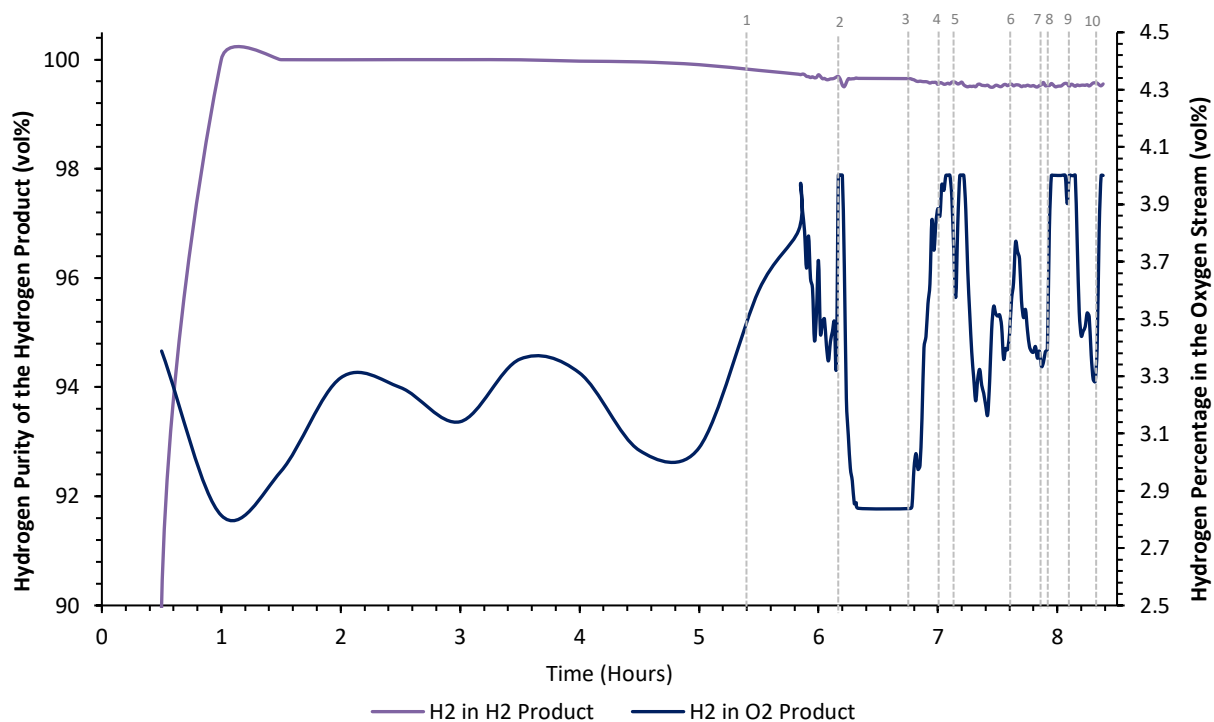


Figure 5-21: Purity Data (vol%) for Purity Degradation Test 3 for the DEFT™ 2.5 unit

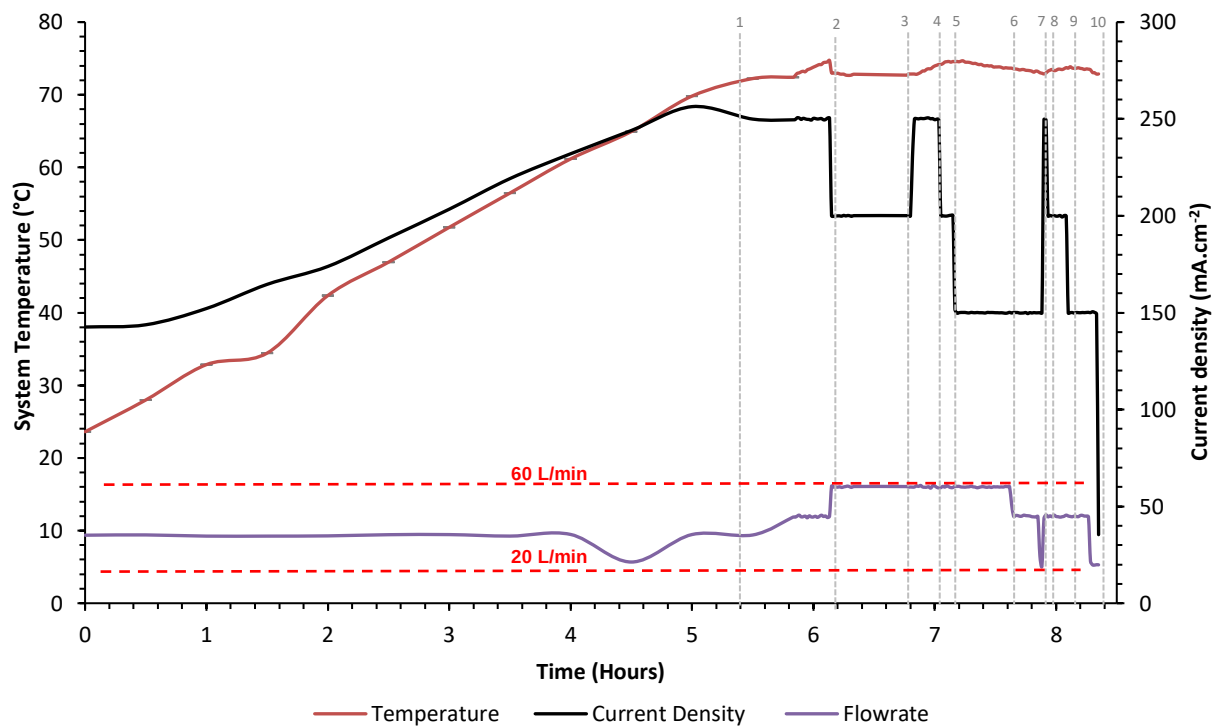


Figure 5-22: Current density ( $\text{mA}\cdot\text{cm}^{-2}$ ), operating temperature ( $^{\circ}\text{C}$ ) and electrolytic flow rate ( $\text{L}\cdot\text{min}^{-1}$ ) data for Gas Purity degradation Test 3

It was observed that low current densities and high electrolytic flow favoured the degraded DEFT™ stack. Recovering the oxygen purities once a contamination level of  $\geq 4$  vol% is reached becomes increasingly difficult.

**Table 5-6: Effects on gas purity with varied operating parameters for Gas purity Degradation Test 3**

| Conditions                       | Change in parameter                               | Effect on O <sub>2</sub> purity | Effect on H <sub>2</sub> purity                                                                                                                                                                  |
|----------------------------------|---------------------------------------------------|---------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| HIGH FLOW + HIGH CURRENT DENSITY | Increasing current density at constant high flow. | Relatively fast degradation     | Effects on H <sub>2</sub> purity remain negligible throughout the test. A slight degradation occurred throughout the test. The H <sub>2</sub> purity remained above 99 vol% throughout the test. |
|                                  | Increasing flow at constant high current.         | Gradual improvement             |                                                                                                                                                                                                  |
| HIGH FLOW + LOW CURRENT DENSITY  | Decreasing current density at constant high flow. | Significant improvement         |                                                                                                                                                                                                  |
|                                  | Increasing flow and decreasing current.           | Significant rapid improvement   |                                                                                                                                                                                                  |
| LOW FLOW + LOW CURRENT DENSITY   | Decreasing current at constant low flows.         | Rapid improvement               | Effects on H <sub>2</sub> purity remain negligible throughout the test. A slight degradation occurred throughout the test. The H <sub>2</sub> purity remained above 99 vol% throughout the test. |
|                                  | Decreasing flow at constant low flow.             | Slight, gradual degradation     |                                                                                                                                                                                                  |
| LOW FLOW + HIGH CURRENT DENSITY  | Increasing current at constant low flow.          | Severe, rapid degradation       |                                                                                                                                                                                                  |
|                                  | Decreasing flow at constant high current.         | Severe degradation              |                                                                                                                                                                                                  |

Table 5-6 indicates that the best remedial action to correct the poor gas was to decrease current densities and increase electrolytic flows simultaneously. Increasing electrolytic flow aids in the separation of the product gases, as dictated by the DEFT™ principle, while decreasing the current density reduces the volume of product gas formed, hence reducing cross-gas contamination. This indicates that the non-conductive layer is inadequately preventing cross-contamination at the reduced flows. As such, the best operating conditions for the degraded DEFT™ stack is low current densities and high electrolytic flow. This suggested that either the non-conductive layer had degraded with operation, or that the electrodes moved out of place to dislodge the non-conductive layer. Operating at low current densities and high electrolytic flow will result in an inefficient (high parasitic load contributions) and expensive system (large stacks) that is highly sensitive to changes in operating conditions. If the non-conductive layer had degraded with time alternative materials that are more resistant to the corrosive alkaline environment could be sourced as the material selection is irrelevant to the operating principle as long as the aperture ratings can be maintained. Alternatively, an investigation was carried out to assess if the position of the electrodes and non-conductive layer had moved out of place over time.

#### 5.4.2.4 Gas Purity Degradation Test 4 – Addition of Locking Ring to the Electrode Assembly.

On removal of the electrolyser stack, all interlocking components were assessed for any indication of degradation/change. It was noted that some of the locking rings, which lock the electrode and non-conductive layer into the housing plate through a press-fit design, had shrunk over time. This resulted in sections of the electrodes not being pressed against the non-conductive layer and hence providing a means for gas to by-pass the non-conductive layer to enter the electrode gap. An additional locking ring was added to the electrode assembly and in this manner the ring formed a press-fit design between the bipolar plant and electrode housing, therefore providing no room for movement. To determine if the observed degradation in gas qualities were due to movement of the electrode or degradation of the nylon/non-conductive separator, additional stability tests were performed. The following results, provided in Figure 5-23 and Figure 5-24, were obtained after the additional locking ring was installed.

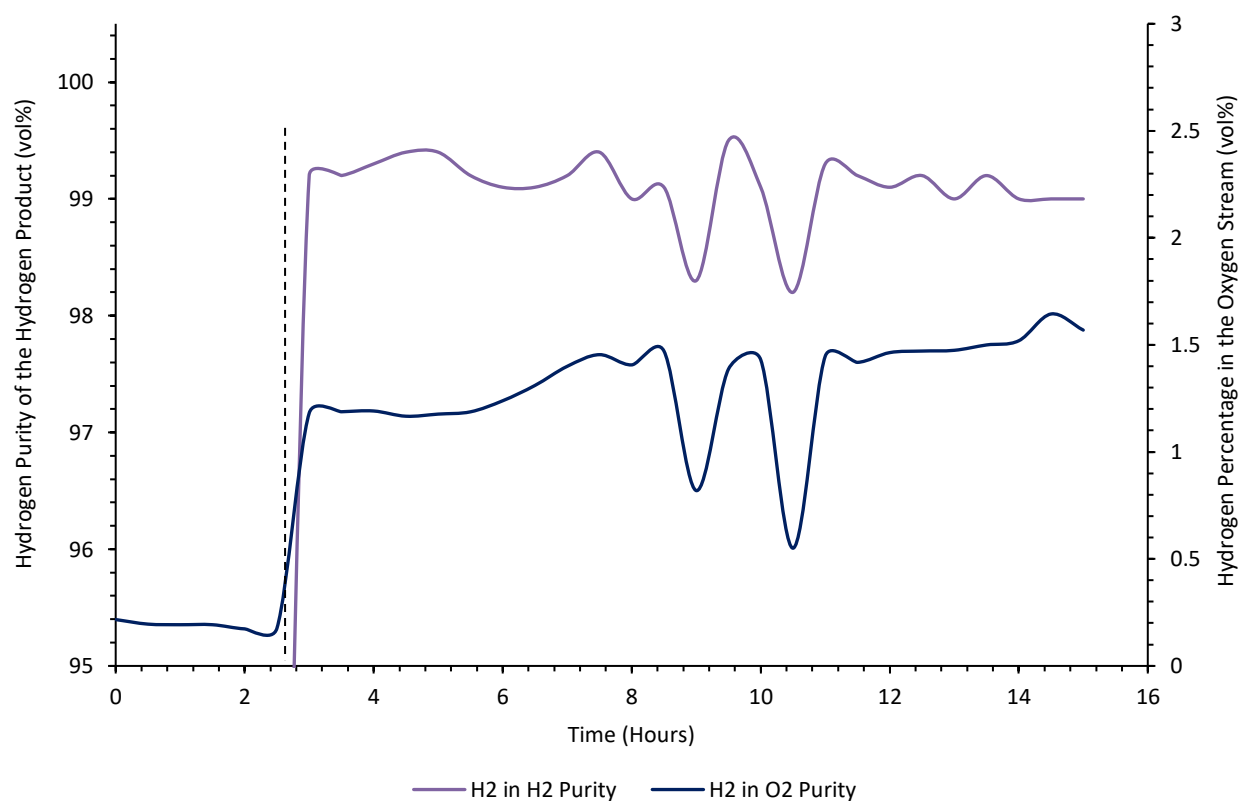


**Figure 5-23: Purity data (vol%) after the addition of locking ring – Gas purity degradation test 4 for DEFT™ 2.5 unit.**

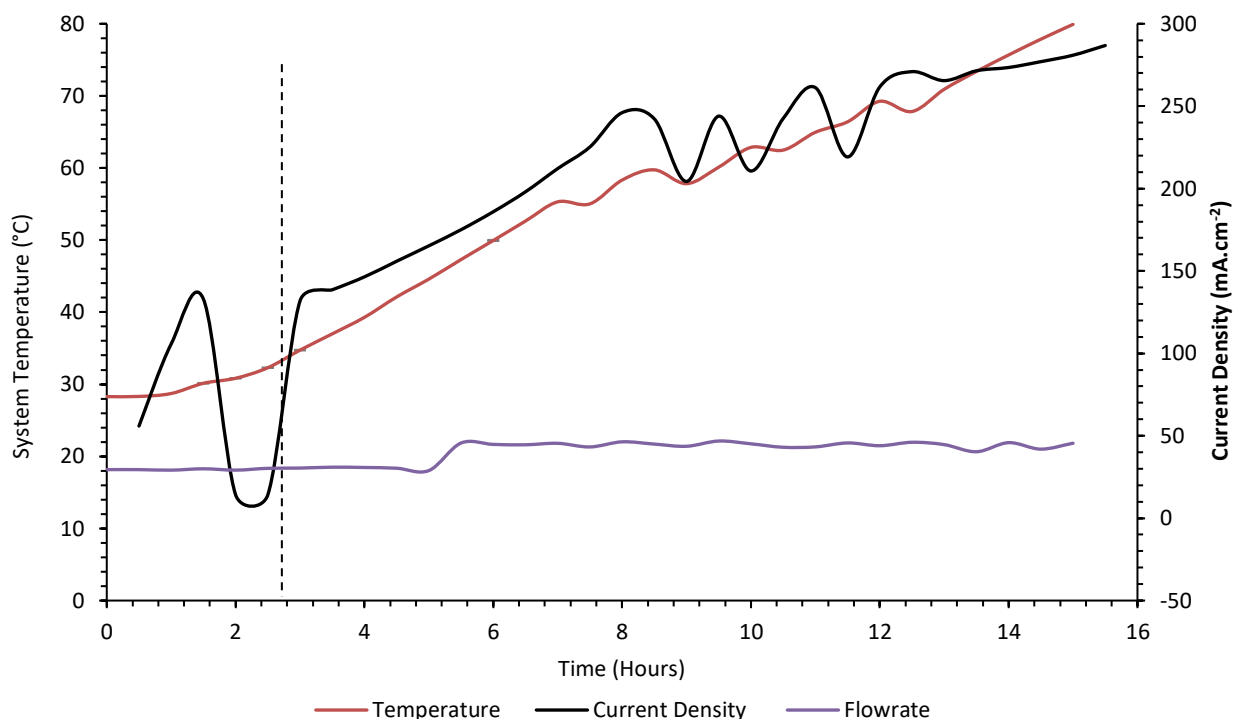


**Figure 5-24: Current supplied (A), Temperature (°C) and electrolytic flowrate (L/min) for Gas Quality degradation Test 4.**

The sampling panels leading to the gas purity meters for both hydrogen and oxygen respectively were opened at ~ 2.5 hours into the test. The electrolytic flowrate through the system was held at ~ 45 L.min<sup>-1</sup> for the duration of the test, while the plant was allowed to heat up to a maximum temperature of 80°C.

The oxygen purities improved significantly, staying within the safe range of operation past a temperature of 60°C. This indicates that cross-gas contamination, due to the movement/dislodging of the electrode, and subsequently, the non-conductive layer, caused a severe degradation in the purity of the oxygen product. With the installation of the additional locking ring, the electrode and the non-conductive layer was secured sufficiently, preventing further cross-contamination. It was therefore concluded that the observed degradation in the qualities of gas products during the 80°C tests was due to the configuration of the electrode assembly, rather than the degradation of the nylon separator material.

The hydrogen gas purity was observed within the range of 98.8 to 99.5 vol% with no notable deviations from previous data before the addition of the second locking ring. This was expected as nylon material used for the non-conductive mesh was not changed or hampered in any way. Conditions in the balance of plant, such as operating liquid levels and electrolyte conditions were changed while re-assembling the stack, in comparison to the conditions in the three previous tests, however, this resulted in no substantial changes to the operation of the stack.

### 5.4.3 Confirmation Polarisation Tests

A final confirmation polarisation test was conducted to determine if the performance of the DEFT™ stack had deteriorated after a significant duration of operation (+/- 500 hours). The test was conducted at 80°C and a flowrate of 45 L.min<sup>-1</sup> (0.0002 m.s<sup>-1</sup>). With the results, provided in Figure 5-25 and Figure 5-26.

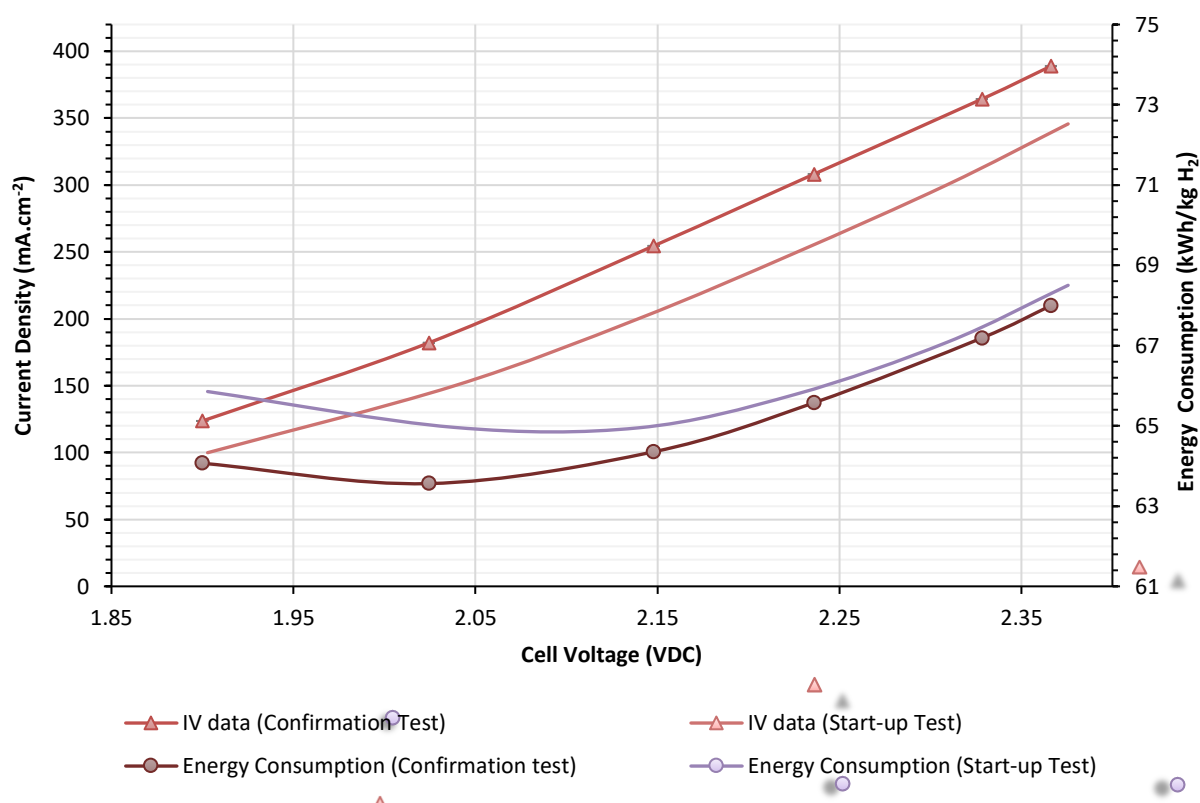


**Figure 5-25: IV and Energy Consumption Data for Confirmation Polarisation test @ 80°C.**

A significant improvement in the current densities achieved by the DEFT™ 2.5 stack was observed during the confirmation polarisation test, with a mean current density increase of roughly 22%. It is believed that this performance improvement is a result of the installation of an additional locking ring to the electrode assembly configuration. The addition of the second locking ring ensured the electrodes were well pressed into the electrode housing, therefore, the electrode gap is maintained at its minimum within each electrode cell. As such, an improvement in the current density, and subsequently, the energy consumption was observed.

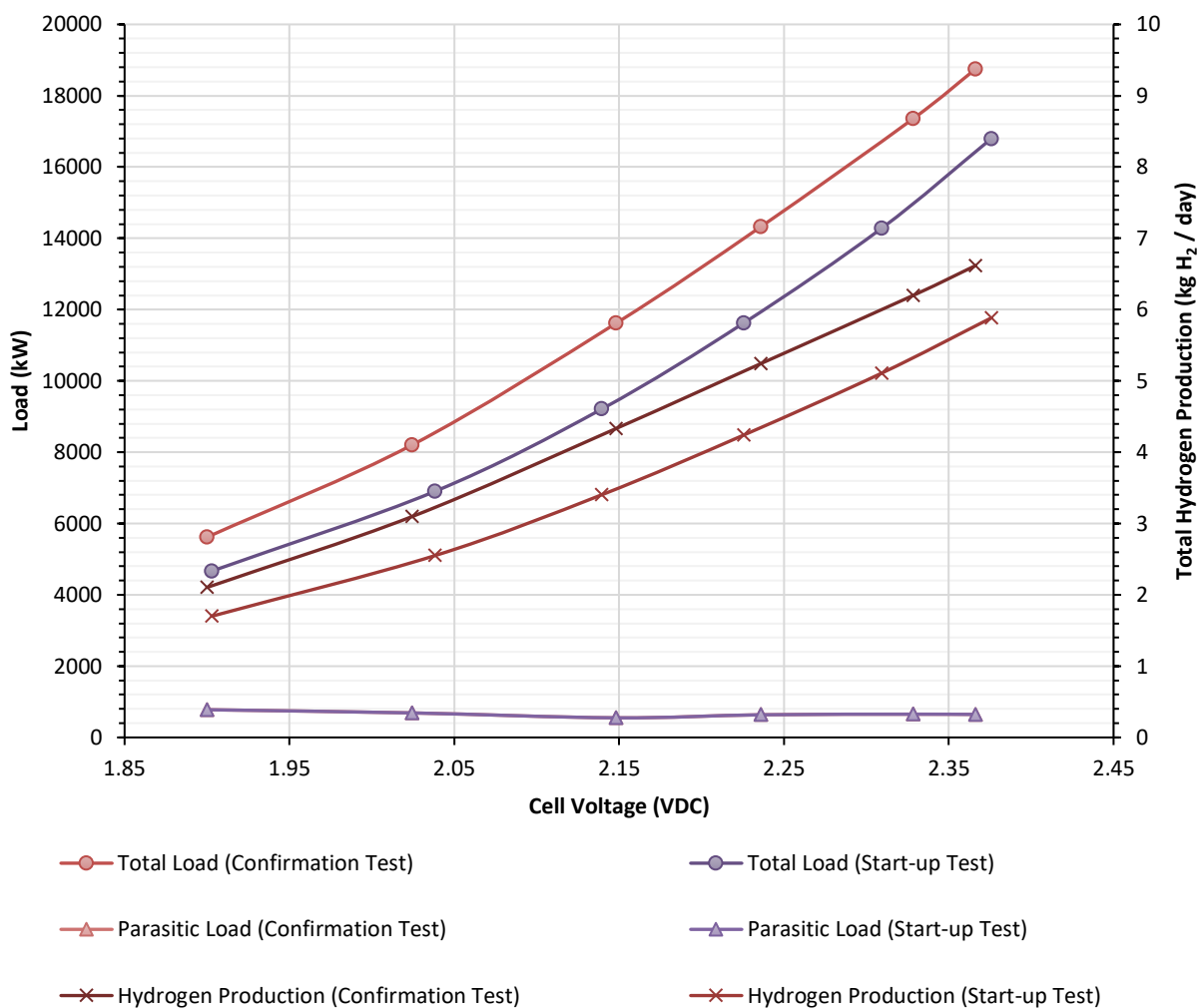


**Figure 5-26: Energy Data for Confirmation Polarisation Test @ 80°C.**

The system load on the stack with the addition of the locking ring resulted in a higher system load, due to the improved current densities. As a result, hydrogen production increased significantly, with a higher amount of hydrogen being produced during the confirmation polarisation test.

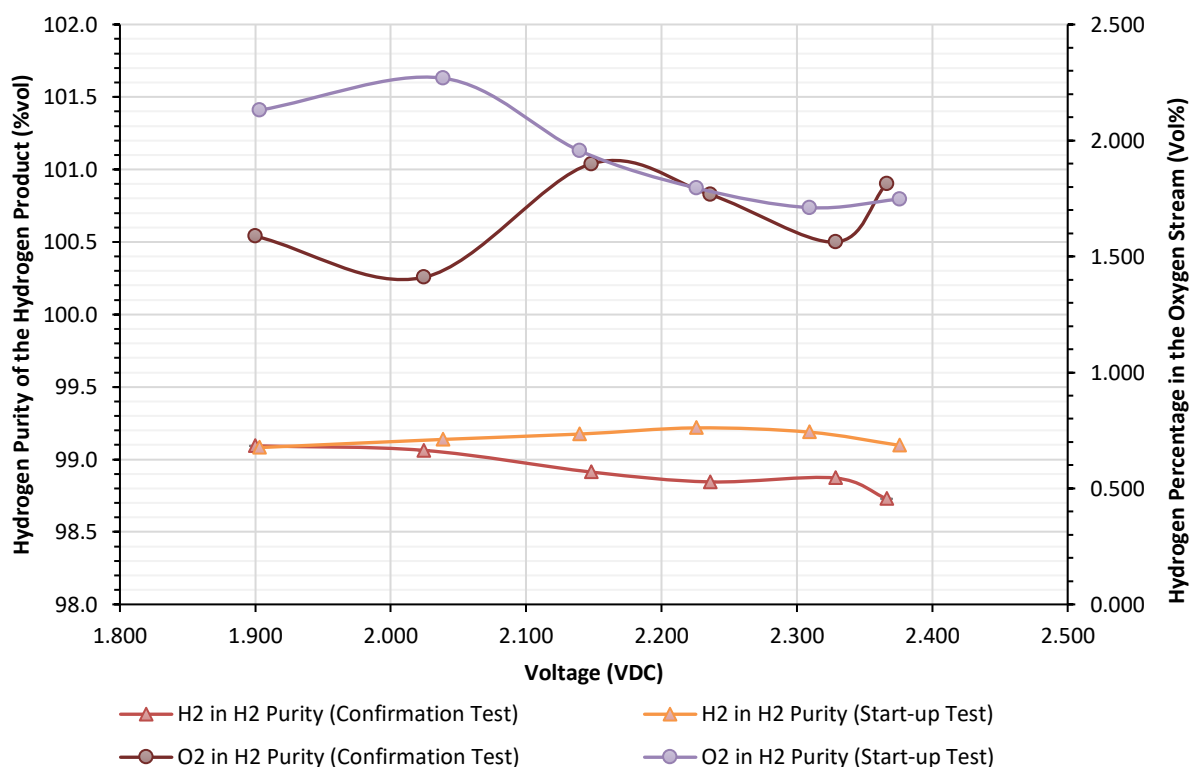


**Figure 5-27: Gas Purity Data for Confirmation Polarisation Test @ 80°C.**

The addition of the locking ring resulted in a significant improvement in the oxygen purities, confirming that the nylon non-conductive layer, coupled with the lower electrolytic flowrate, is capable of preventing significant amounts of cross-gas contamination at the higher end of the chosen electrolytic flow velocities for the DEFT™ 2.5 unit.

**Table 5-7: Performance improvements of the DEFT™ system - confirmation tests vs start-up tests @ 80°C and 45 L.min<sup>-1</sup>**

| System Improvements       |                 |
|---------------------------|-----------------|
| Current Density           | 12.5 % to 27.2% |
| System Energy Consumption | -0.2% to - 2.7% |
| Hydrogen Purity           | -0.38% to 0%    |
| Oxygen Purity             | -4% to 38%      |

#### **5.4.4 Comparison of DEFT™ to a Similar Zero-Gap Configuration**

As previously mentioned, the nature of the DEFT™ 2.5 plant's operating principle requires that tolerance concerning high solution flows and potential impure gas purges would need to be allowed for and incorporated into the system. This would prove not to be a problem, however, the technology then needs to demonstrate some key advantage either in terms of performance, cost, or niche application over commercially available technologies to encourage its uptake in the market. Throughout the dissertation, a comparison is made between the associated cost and performance of a conventional system to the DEFT™ technology. The DEFT™ reactor remains largely unoptimised from a catalytic, configuration and general structural perspective and hence making comparisons to conventional systems, which have these aspects incorporated (i.e. catalytic coatings, etc.) would result in an unfair and inaccurate comparison. Comparisons to conventional technologies would require like for like comparisons. Consequently, tests were structured with the intended purpose of providing a direct comparison between a Zero-Gap configuration making use of Zirfon ULP500 and that of the DEFT™ configuration utilising the 5 µm mono-filament nylon material. Configurations on all accounts make use of the same spacer, electrode and pre-electrode material except for the configuration being either DEFT™ or Zero-gap and the selected separator material. The tests were performed on the 230 mm Bipolar Bi-MCFP prototype, shown in Figure 5-1, with a single cell. The single-cell configuration was chosen to allow for a simple modification to a zero-gap design. In this case, the central manifold threads, as per Figure 5-4, were removed allowing for installation of a Zirfon Perl® diaphragm. The results collected for these comparisons are depicted in Figure 5-28.

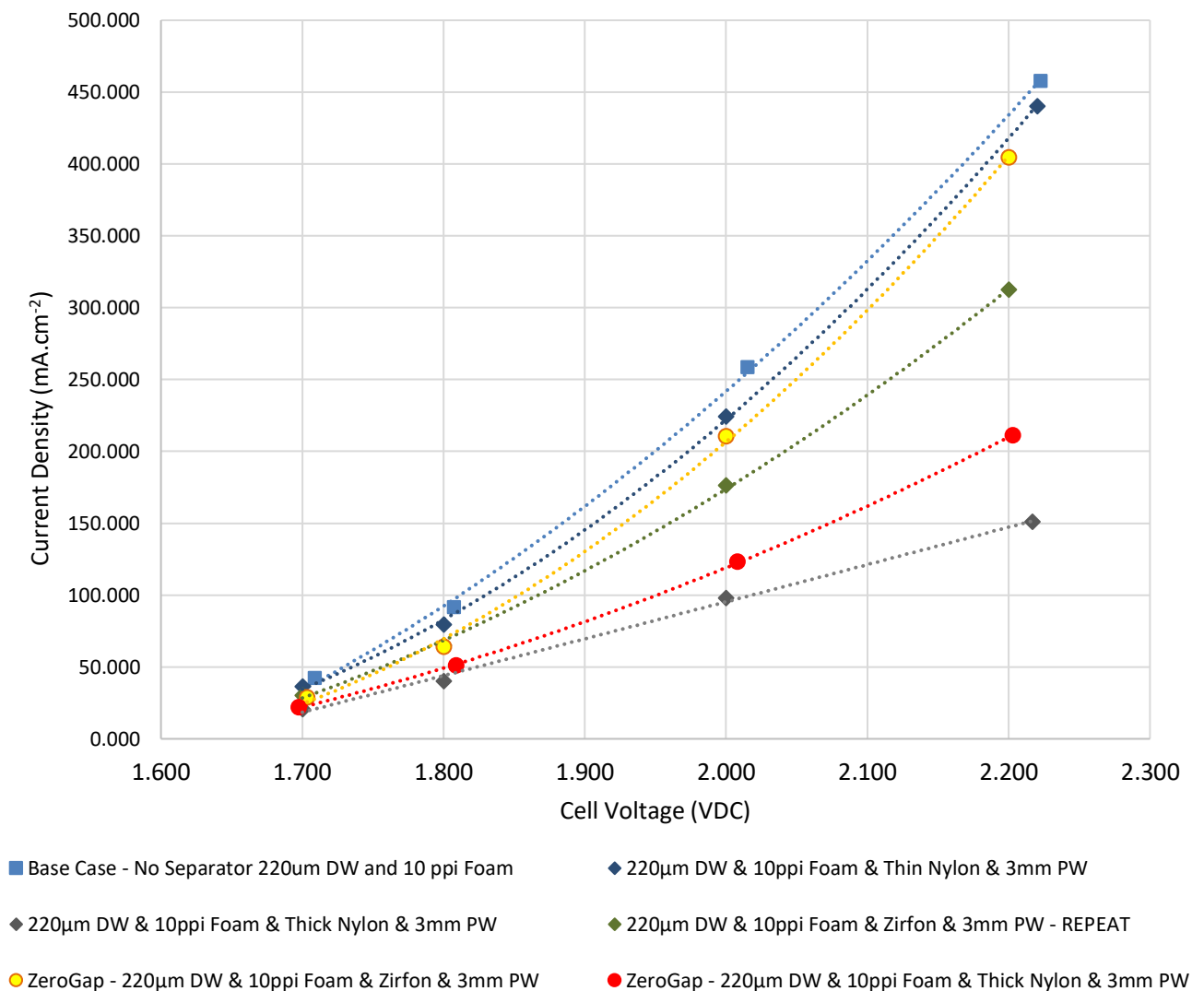


**Figure 5-28: IV curves for a variety of DEFT™ and Zero-Gap configurations at an electrolytic concentration of 30 wt% KOH, a system temperature of 65°C and cross-sectional electrolytic flow velocity of 0.002 m.s<sup>-1</sup> (DW -Dutch weave, PW – plain weave).**

It is immediately apparent that, with an electrode gap present, the base case configuration making use of no separator (light blue square) and that of the thin nylon DEFT™ configuration (dark blue diamond) shows good agreement in performance. A mean percentage loss in current density of 25% is noted between the base case and operation with the 5 µm non-conductive mesh, which is in agreement with the values determined earlier and presented in Table 3-3. This indicates that the incorporation of the mono-filament nylon separator material adds to the resistance of the cell, however, it does not prove to be detrimental to the cells operating performance as current densities above that of zero-gap configurations are still noted. By improving the separation efficiency within the reactor and simultaneously moving toward lower electrolytic fluid flows by

including thicker multi-filament nylon into the configuration, adds significant resistance to the cell as illustrated by the grey diamond curve. This is further exemplified when examining the performance of thick multi-filament nylon installed in a zero-gap configuration (Red circle). Zirfon Perl ULP500 is a material developed by AGFA for the alkaline water electrolysis industry as to function as a highly efficient separator, which acts as a conductive transport medium for ions. By incorporating this material into the DEFT™ configuration (green diamond) it is possible to see the effect of the resistance added to the cell when compared to the monofilament nylon and base case conditions.

The interesting observation concerning Figure 5-28 is the comparison of monofilament nylon (dark blue diamond) to that of a zero-gap system utilising a Zirfon Perl separator (Yellow circles). It is observed that DEFT™ provides higher performance showing 10 – 42% higher current densities at set voltages. This indicates that at the stipulated conditions the DEFT™ 5 µm non-conductive configuration results in lower cell resistances compared to a zero-gap Zirfon Perl setup. This result proves promising as the DEFT™ technology could, for example, potentially be configured to achieve even higher current densities when subjected to higher temperature operation which is not possible with a conventional separator setup. The additional attributes concerning parasitic loads and purge gas creation would be worth addressing as the technology would now be amended to an advanced operational state (i.e. higher current densities and stack efficiencies), with this state now motivating a competitive OPEX and CAPEX case for the technology.

## 5.5 Conclusion

The DEFT™ 2.5 system was able to meet many of the soft targets outlined in Section 1.2.2. Table 5-8 provides the outcomes of these performance targets (excluding economic targets).

**Table 5-8: Project soft targets and DEFT™ 2.5 outcomes at an operating temperature of 80°C and a flowrate of 45 L.min<sup>-1</sup>.**

| Project Targets                                                                                         | DEFT™ 2.5 Outcomes                                                                                                                                                                                                                                                        |
|---------------------------------------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 1. An overall system energy consumption of <b>90 kWh/kg H<sub>2</sub></b> (higher heating value basis). | The DEFT™ 2.5 unit was able to achieve efficiencies between <b>64 – 68 kWh/kg H<sub>2</sub></b> over a range of <b>1.8 – 2.4 VDC</b> respectively. These values were obtained at an operating temperature of 80°C and a flowrate of ~45 L/min (0.0002 m.s <sup>-1</sup> ) |

3. An efficient and reliable gas/liquid separation system capable of yielding H<sub>2</sub> and O<sub>2</sub> purities of **>99.5 vol%**.

Hydrogen purities of **> 99.5 vol%** were achieved **at flowrates of 45 L/min and greater**, however, steady-state hydrogen gas purities fell within the **98.5 – 99.5 vol% range**. Oxygen purities were kept within the safe operating range (>94 vol% H<sub>2</sub> [104]) by installing an additional locking ring to the electrode assembly.

The **% purge** (w.r.t hydrogen product) was decreased to **0.88% - 3.1%**, but was not entirely removed from the system.

4. A **scalable reactor** design capable of complying with the overall energy consumption and gas purity targets

The current design of the DEFT™ 2.5 system requires further development to overcome **flow path and flow distribution limitations** to achieve successful scale-up.

5. Reduction in parasitic loads to be **< 35%** of the total plant energy consumption

Parasitic loads were reduced to a range of **3.2 – 13.5% (of which pumping accounts for 1.9 – 7.5%)** for an operating voltage of 1.8 – 2.4 respectively.

In its current configuration the technology, however, still struggles to meet objective 4 in its entirety. Scaling the technology to larger electrode sizes would require further flow reductions. Reference to Figure 5-26, the confirmation test at 2 VDC, a total plant load of 11.6 kW is noted at a flow rate of ~45 L/min. To scale this directly to a 100 kW scale system a flow rate of 388 L/min would still be required. Furthermore, maintaining a uniform flux distribution across a larger electrode surface would remain challenging.

Although long term stability tests on the DEFT™ system were not formally conducted, the average operating time taken to operate the unit and collect the data presented in this dissertation totalled to ~ 500 hours of operating time. Confirmation polarisation tests were conducted thereafter to assess the performance of the DEFT™ stack.

Even with the installation of an additional locking ring, a small percentage of purge gas was still produced from the DEFT™ 2.5 system. The purge production rate equated to approximately 0.8% - 3.1% of the hydrogen product output. Although the percentage purge (w.r.t hydrogen product) is relatively low, it is still desirable that no purge is present, as this will become a more pressing issue with scale-up. Table 5-9 provides an updated version of Table 3-6 which includes a summary of the Bipolar Bi-MCFP stack.

**Table 5-9: Comparison of the Bipolar Bi-MCFP, Bi-MCFP, and MCFP prototype**

| Parameter                                                             | Bipolar Bi-MCFP | Bi-MCFP | MCFP [1] |
|-----------------------------------------------------------------------|-----------------|---------|----------|
| Voltage (VDC)                                                         | 2.0             | 2.0     | 2.0      |
| Temperature (°C)                                                      | 60              | 60      | 60       |
| Current Density (mA.cm <sup>2</sup> )                                 | 130             | 104     | 578      |
| Flowrate velocity (m.s <sup>-1</sup> )                                | 0.0002          | 0.001   | 0.075    |
| Required cathodic electrode area for 5 kg/day H <sub>2</sub> capacity | 4.3             | 5.3     | 0.96*    |
| Flowrate required for 5 kg/day H <sub>2</sub> capacity                | 102             | 635     | 8 625*   |
| Pump and stack energy consumption                                     | 55.9            | 71.4    | 144.2*   |
| % parasitic load                                                      | 4.6             | 25.3    | 63*      |

\* Calculated under the assumptions listed in Section 3.3.3

Table 5-9 provides power consumption estimations for the Bipolar Bi-MCFP, Bi-MCFP, and MCFP prototypes under the assumptions listed in Section 3.3.3. The power consumption values provided includes the power consumption of the stack and pump and not that of the BOP and AC to DC rectifier efficiency in order to provide a like for like performance comparison irrelevant of the balance of the plant in which the electrolyser stack was installed. With a rectifier efficiency of 92% the 55.9 kWh/kg H<sub>2</sub> value increase to 60.76 kWh/kg H<sub>2</sub>. With the inclusion of BOP power and AC to DC rectifier efficiency the power consumption increase to roughly 68 kWh/kg H<sub>2</sub> at 60°C and 0.0002 m.s<sup>-1</sup> as per the values reported in Figure 5-9.

The DEFT™ 2.5 unit, in its current configuration, is not suitable for industrial scale-up, due to its flow path limitations. Fluid injection through the centre of the stack allows for results in limited flow distribution across the surface of the electrode. Furthermore, the radial injection of electrolyte from the centre of the stack creates a larger flow distance, hence hampering flow distribution. To achieve feasible scale-up of the DEFT™ technology, further developments must be made to the electrolyte injection methods and the electrode assembly configuration.

Furthermore, the overall system efficiencies achieved by the DEFT™ 2.5 unit, while meeting the objectives listed in Section 1.2.2, did not prove to be competitive against the performance achieved by industrial competitors. No additional benefit of operating with the enhanced electrolytic flow over conventional operation was observed in the performance. While a slight reduction in the CAPEX of the plant was achieved, this was due to the cost savings associated with the removal of conventional membranes and an efficiently designed plant. It is important to note, however, that the DEFT™ 2.5 system was unoptimised and can be improved to match industrial standards in terms of performance through further development of catalyst and the electrode assembly.

## CHAPTER 6 - DEFT™ TECHNOLOGY PILOT TECHNO-ECONOMIC ASSESSMENT

### 6.1 Overview

The DEFT™ 2.5 unit was designed and manufactured as part of Phase 3 of the project. The objective of this project was to design and fabricate an electrolysis unit demonstrating the DEFT™ operating principle on a small scale. A techno-economic analysis was conducted to determine whether the DEFT™ 2.5 unit showed any economic viability for market introduction. The economic objective of the project was noted as:

Hydrogen costs < **7.5 \$/kg H<sub>2</sub>**, with the CAPEX of DEFT™ units < **5 \$/kg H<sub>2</sub>** for small scale production (<20 kg/day).

The design of the DEFT™ 2.5 unit was focused on producing a low-CAPEX unit, at the targeted production rate of 5 kg/day H<sub>2</sub>. As such, cost-effective materials were investigated for the design of the unit, and local manufacturers were used to fabricate the electrolyser stack and balance plant.

The intention behind the design of the DEFT™ 2.5 plant, was to produce a pre-commercial unit that would exhibit the potential for commercial use and possible scale-up. Not only will the design and operating principle of the DEFT™ 2.5 unit be analysed, but also the capability of the unit to achieve the desired operating conditions at a reduced system CAPEX and OPEX, in comparison to industry. For the development of a commercial representative pilot a fully integrated and automated system needed to be designed and commissioned. Phase 2 of the project, was dedicated to the development of a control and operating procedure. This included the design of power and control circuits as well as the determination of PLC I/O's (inputs and outputs). With the development of a working P&ID document, an internal and external HAZOP review was undertaken. The work and investigations surrounding phase 2 developments have not been provided in this report, however, it is worth noting that these processes were carried out not only to ensure the safe operation of the pilot plant but also to ensure that the engineering and development work was representative of a commercial project undertaking. This ensured that the pilot plant incorporated the necessary instrumentation and auxiliary units required for the demonstration to be considered as a representative commercial system thus incorporating the costs and power consumption associated with plant automation, additional layers of safety, etc., that would otherwise have been excluded in the development of an experimental test rig.

## 6.2 Costing Methodology

The costing analysis for the DEFT™ 2.5 unit was conducted in three phases:

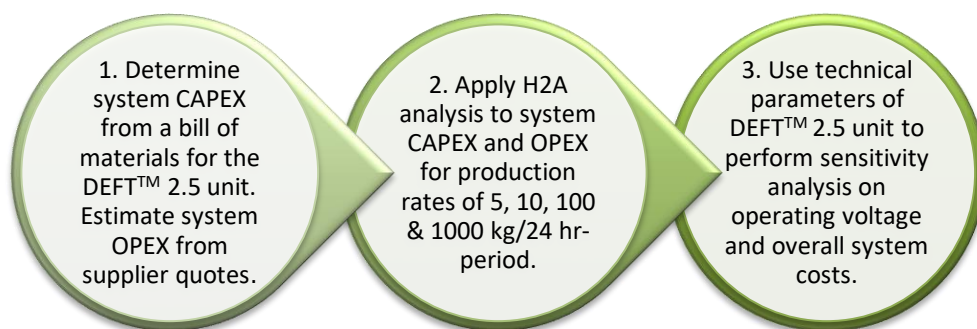


**Figure 6-1: DEFT™ 2.5 costing analysis process**

This analysis was conducted for five different system configurations:

- 1) Generation of H<sub>2</sub> only at atmospheric pressure (Purity >99.5 Vol%) for the R&D model.  
**(R&D)**
- 2) Generation of H<sub>2</sub> only at atmospheric pressure (Purity >99.5 Vol%) on a commercial basis.  
**(Production Only)**
- 3) Generation of H<sub>2</sub> only at atmospheric pressure (Purity >99.995 Vol%) for a Client.  
**(Production & Purification)**
- 4) Generation of H<sub>2</sub> only at compression up to 200 bar (Purity >99.5 Vol%) for a Client.  
**(Production & Compression)**
- 5) Generation of H<sub>2</sub> only at compression up to 200 bar and purification to >99.995 Vol% for a client. **(Production, Compression & Purification)**

Points 3 – 5 were based on the theoretical compression and purification of the hydrogen product. The parameters associated with the compression and purification systems were found in literature and used to predict cost and performance figures for the DEFT™ technology in its current form. To determine the cost of a commercial unit, the equipment and instrumentation pieces on the R&D model required for testing, were removed from the bill of materials and listed as a possible saving. This included the removal of one-off costs that were not considered to be direct costs such as the cost of PLC coding, the generation of fabrication drawings, etc. A detailed breakdown of these savings can be found in the CAPEX analysis section, (Section 6.3.1).

### 6.2.1 Costing Analysis Assumptions.

The following assumptions were made when conducting the costing analysis:

- The scaling factors used in the H2A analysis, detailed in Section 6.2.3, were assumed accurate and applicable to the CAPEX and maintenance OPEX of the plant. The scaling factors were obtained from the Wind-To-Hydrogen project report by G. Saur [18].
- The Rand-Dollar exchange rate used was R14 to \$1.
- The cost of electricity used by the plant as well as the R-\$ exchange rate would remain constant throughout the life of the plant and fluctuations in price were not considered.
- Maintenance estimations were made using recommendations and quotes for consumables from suppliers.
- Estimations regarding CAPEX savings were made when calculating the cost in the commercialisation of the plant, provided in Section 6.3.1.
- An operating year was assumed to be 362 days, with 3 days being set aside for maintenance of the unit.
- The plant lifetime was assumed to be 20 years.

### 6.2.2 Costing Procedure

1. The bill of materials for the current 5 kg/day H<sub>2</sub> test plant was used to determine the initial CAPEX for the plant. The OPEX of the plant was determined using estimations regarding consumables and frequency of maintenance.
2. The savings associated with removing the R&D cost for a commercial system was estimated. This results in a lower system CAPEX for the streamlined, commercial DEFT™ unit and was noted as “Production only” costs.
3. The operating efficiency of the plant was determined through polarisation tests conducted on the DEFT™ 2.5 unit, outlined throughout Section 5. The operating efficiency was used to obtain the kW rating of the unit at different operating voltages/efficiency ratings. The CAPEX/kW<sub>installed</sub> and OPEX/kW<sub>installed</sub> values were then determined for the unit.
4. CAPEX/kW<sub>installed</sub> and OPEX/kW<sub>installed</sub> values were inputted into the H2A model to determine CAPEX and OPEX data for the DEFT™ unit at production rates of 5, 10, 100 and 1000 kg/day H<sub>2</sub> respectively. The H2A model will be further discussed in the following sections. The kW<sub>installed</sub> data was then used to determine total CAPEX and OPEX values for larger-scale systems.

5. Technical parameters obtained from polarisation data for the DEFT™ 2.5 unit were used to conduct a sensitivity analysis on the voltage and total system costs for production rates between 5 – 1000 kg/day H<sub>2</sub>.
6. Cell potentials were varied between a range of 1.8 to 2.4 VDC, and stack size was changed accordingly to maintain a production rate at 5 kg/day H<sub>2</sub>. Cost data was then calculated for the various operating cell voltages. A 5 kg/day H<sub>2</sub> rate of production was therefore used as a basis for this cost study.
7. The total lifetime production of hydrogen and kWh consumption for the DEFT™ 2.5 unit was determined. The lifetime electrical costs were then determined using an electricity price of 0.07 \$/kWh, obtained from a grid-solar combination system. This was done for the stipulated operating cell voltages.
8. Costs per kilogram of hydrogen were then determined for CAPEX, OPEX, and electrical expenses; the total lifetime production of hydrogen was used to calculate the \$/kg H<sub>2</sub> values for the stipulated operating voltages.
9. The cost data obtained from the analysis was then used to determine the performance of the DEFT™ 2.5 plant at various production scales against the economic objective (Hydrogen costs < 7.5 \$/kg H<sub>2</sub> and CAPEX < 5 \$/kg H<sub>2</sub>), and industrial standards.

### 6.2.3 H2A Model and Ivy & Saur Analysis

The method used to determine the CAPEX and OPEX (\$/kW<sub>installed</sub>) for scaled systems, with the DEFT™ 2.5 unit as a basis, was derived from reports released by the National Renewable Energy Laboratory (NREL), namely, Wind-To-Hydrogen Project by G. Saur and Summary of Electrolytic Hydrogen Production by J. Ivy [17], [18]

The H2A model accounts for the depreciation in capital costs using the MACRS (Modified Accelerated Cost Recovery System) standard economic model. The H2A study performed by NREL led to the comprehensive accumulation of data from various systems which allowed for the determination of the total CAPEX costs for electrolysis systems as a function of the rate of production. An equation trend was applied to this data and the following equation, Eq. 6-1, was the result thereof [18]:

$$y = 224.49x^{0.156} \quad \text{Eq. 6-1}$$

where:

x = Production rate (kg H<sub>2</sub>/hr)

y = Total CAPEX cost of the electrolysis system in 10<sup>3</sup> US dollars.

The H2A study then assumed an efficiency to determine installed CAPEX figures (US \$/kW<sub>installed</sub>) for an efficiency of 63 HHV% or energy consumption of 62.8 kWh/kg H<sub>2</sub>. From this model, Table 6-1 shows the expected costs of electrolysis units at the respective production rates.

**Table 6-1: Capital costs used in H2A analysis [18].**

| Production Rate<br>(kg/24 hrs) | X Variable<br>(kgH <sub>2</sub> /hr) | Electrolyser CAPEX<br>(\$) | Electrolyser CAPEX<br>(\$/kW <sub>installed</sub> ) |
|--------------------------------|--------------------------------------|----------------------------|-----------------------------------------------------|
| 10                             | 0,42                                 | 131 604                    | 5000                                                |
| 100                            | 4,2                                  | 543 087                    | 2000                                                |
| 1000                           | 42                                   | 2 241 141                  | 850                                                 |

The study indicates the cost of electrolyser systems and changes in said costs with economies of scale. The DEFT™ technology, however, has its unique CAPEX considerations, therefore, the CAPEX estimations provide by NREL would not be useful for this study. The changes in costs (scaling factor) does, however, provide a useful indication of how the costs of the DEFT™ technology would potentially benefit with economies of scale. These scaling factors were obtained from the NREL data by determining a cost savings factor by dividing the costs of a 10 kg/day H<sub>2</sub> system (as per Eq. 6-1) by costs for larger capacity plants. The result of this is provided in Figure 6-2.

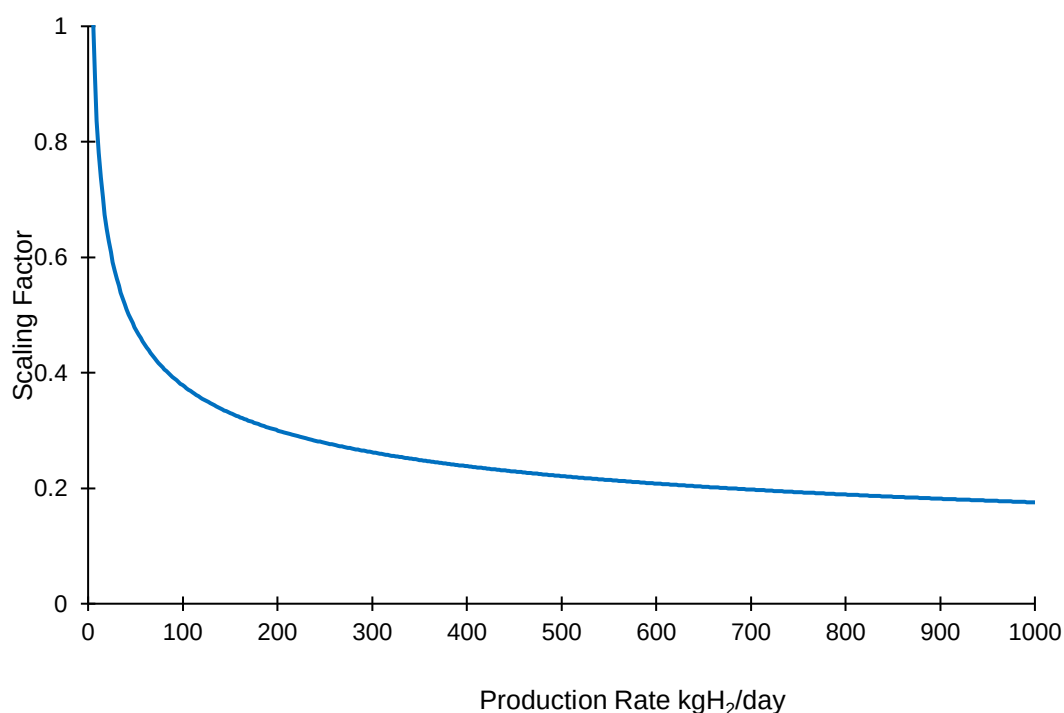


**Figure 6-2: Cost Scaling factors versus Production Rate.**

From Figure 6-2, Eq. 6-2 was developed, which relates the scaling factors to various production rates:

$$y = 1.7518x^{-0.333} \quad \text{Eq. 6-2}$$

where:

x = Production Rate (kgH<sub>2</sub>/day)

y = Scaling Factor

The scaling factors used for the various production rates may be found in Table 6-2.

**Table 6-2: Cost scaling factors at various production rates**

| Production Rate (kgH <sub>2</sub> /day) | Scaling Factor |
|-----------------------------------------|----------------|
| 5                                       | 1              |
| 10                                      | 0.814          |
| 100                                     | 0.4            |
| 1000                                    | 0.17           |

## 6.3 Results and Discussions

### 6.3.1 CAPEX Data for the DEFT™ 2.5 Unit

The CAPEX for the DEFT™ 2.5 unit was determined by considering the costs for the design and manufacturing of the R&D model of the plant. Costs for gas purification and compression were also considered when calculating the system CAPEX. The test rig that was built (identified as the R&D model) does not, however, contain purification and compression equipment. A detailed breakdown of the system R&D CAPEX costs for the DEFT™ 2.5 unit can be found in Appendix E.

To estimate the costs representative of a commercial system through removal of the R&D and once-off costs, i.e. the 'Production Only' unit model, several modifications were applied to the cost analysis of the R&D model. These modifications included removing any unnecessary equipment that would not be required in a commercial electrolysis unit, removal of once-off costs and streamlining some design procedures. A breakdown of the savings incurred by the suggested optimizations and associated changes can be seen in Table 6-3.

**Table 6-3: CAPEX savings for a commercial DEFT™ 2.5 unit.**

| Item                                    | Savings            | Motivation for Savings Estimate                                                              |
|-----------------------------------------|--------------------|----------------------------------------------------------------------------------------------|
| Liquid Flow Meter                       | \$433,65           | Replaced analogue flow meter with a more cost-effective flow switch                          |
| KOH Conductivity Sensor                 | \$560,93           | Removal of KOH Conductivity Sensor                                                           |
| Reactor Plastic Components (Outsourced) | \$1 359,21         | 20% saving as no engineering or drafting required in future.                                 |
| Bi-polar plates                         | \$750,00           | 50% savings switching to carbon steel, nickel-plated bi-polar plates.                        |
| Gas-Liquid Separators                   | \$1 495,07         | 20% saving as no engineering or drafting required in future.                                 |
| Gas Washers                             | \$763,79           | 20% saving as no engineering or drafting required in future.                                 |
| Purge Vessel                            | \$210,50           | 20% saving as no engineering or drafting required in future.                                 |
| PLC Programming & Commissioning         | \$4 928,57         | PLC programming & commissioning not required in future.                                      |
| Variable Speed Drive                    | \$1 197,14         | Will not be required on commercial setup                                                     |
| DC Stack                                | \$1 725,00         | Will not require modifications post-production in future.                                    |
| Electrical Design (Labour)              | \$4 435,71         | Will not require future design work.                                                         |
| Framework                               | \$2 228,36         | 50% saving as the frame will not be made from stainless steel                                |
| Framework (Labour)                      | \$1 386,86         | 50% saving as no engineering or drafting required in future and frame can be built in-house. |
| <b>Total Savings</b>                    | <b>\$21 474,79</b> |                                                                                              |

The total savings from the modifications of the system resulted in a 15% drop in the overall cost of the system, including both CAPEX and OPEX and a ~ 28% reduction in the CAPEX of the unit. The DEFT™ 2.5 unit, is, however, still at the pre-commercial stage, and so the system can still be further optimised to improve the system's CAPEX, as well as OPEX values. Table 6-4 shows the CAPEX costs associated with each of the above-mentioned configurations.

**Table 6-4: Total CAPEX costs for various configurations of DEFT™ 2.5 unit.**

| Configuration                          | CAPEX       |
|----------------------------------------|-------------|
| R&D                                    | \$76 157,14 |
| Production Only                        | \$54 682,28 |
| Production & Purification              | \$70 682,21 |
| Production & Compression               | \$66 005,14 |
| Production, Purification & Compression | \$82 005,21 |

An expected increase in the system CAPEX is seen with the addition of the gas compression and purification steps. These cost figures apply to the DEFT™ 2.5 unit which is capable of producing 5 kg of hydrogen at the operating conditions provided in Table 6-5.

**Table 6-5: Operating parameters for DEFT™ 2.5 unit at 80°C.**

| Operating Condition                             | Value           |
|-------------------------------------------------|-----------------|
| Temperature (°C)                                | 80              |
| Pressure (mBar)                                 | ~ 320           |
| Electrical Consumption (kWh/kg H <sub>2</sub> ) | 67.107          |
| System Efficiency (HHV%)                        | 58.71 %         |
| Cell Potential (VDC)                            | 2.328           |
| Current Density (mA/cm <sup>2</sup> )           | 302.362         |
| Production Rate (kg/day H <sub>2</sub> )        | 5.144           |
| Electrolytic Flowrate (l/min)                   | ~ 11.31         |
| Hydrogen Purity (%)                             | 98.892 – 99.227 |
| Purge Gas (% of total flowrate)                 | 0.0033 – 0.0123 |

Based on the operating parameters in Table 6-5, the following cost data, provided in Table 6-6, was derived for the DEFT™ 2.5 plant.

**Table 6-6: CAPEX/kW<sub>installed</sub> and CAPEX/kg H<sub>2</sub> values for various configurations of the DEFT™ 2.5 unit. Values are on an 80°C basis.**

| Configuration                                | Energy Load (kW) | CAPEX/kW <sub>installed</sub> (\$/kW) | CAPEX/kg (\$/kg H <sub>2</sub> ) |
|----------------------------------------------|------------------|---------------------------------------|----------------------------------|
| R&D                                          | 13.97            | 5 447. 91                             | 2,10                             |
| Production Only (P)                          | 13.97            | 3 911.71                              | 1,51                             |
| Production & Purification (PP)               | 17.1             | 4 132.47                              | 1,95                             |
| Production & Compression (PC)                | 15.22            | 4 334.14                              | 1,82                             |
| Production, Purification & Compression (PPC) | 18,35            | 4 467.94                              | 2,26                             |

\* Energy consumption for purification and compression steps were assumed to be 15 and 6 kWh/kg H<sub>2</sub> respectively.

According to Saur, ≤10 kg/day H<sub>2</sub> production systems are found to be ≥ \$ 5000/kW<sub>installed</sub> [18]. Based on the operating efficiency of 62.8 kWh/kg, this equates to a total system CAPEX of \$ 65 416.70 for a 'Production Only' commercial unit. The DEFT™ 2.5 unit, therefore, shows a ~16.4% reduction in CAPEX costs, in comparison to small scale industrial standards. This reduction, however, comes at the expense of lower system efficiencies. According to the sensitivity analysis carried out in Section 6.3.1.3, the CAPEX of a DEFT™ unit at a comparing system efficiency of 62.8 kWh/kg, is ~ 10.7 % higher than industrial standards. Consequently, CAPEX reductions for the DEFT™ unit are only realised at lower efficiencies. This data, however, has been generated with the use of pure nickel electrodes, thus, the system does not work to reduce the cathodic and anodic overpotential through the deployment of a catalyst, or by modifying the current electrode configuration by employing higher active area electrodes. Deployment of a catalyst with a net positive cost to performance characteristic would allow for the reduction in CAPEX to be achieved at the benchmarked efficiencies. The data presented by NREL in the Saur report made use of market surveys to generate data. These entities that form part of this survey would have worked to already include catalytic benefits in their systems. This comparison, however, does provide a representative market positioning of the current DEFT™ configuration. The analysis here could also be used for future benchmarking of catalyst incorporation studies.

#### 6.3.1.1 Economies of Scale

The effect of scale-up of the DEFT™ 2.5 system was investigated on the current DEFT™ 2.5 unit at a system efficiency of that outlined in Table 6-5. Economies of scale as expected, improves the system CAPEX per kW installed. Not only are the system components subjected to the

benefits of economies of scale, but the costs of instrumentation, which remains relatively the same throughout the scale range, is offset by larger production capacities. Figure 6-3 shows the effect of economies of scale on the CAPEX of the DEFT™ electrolyser system at various production outputs.

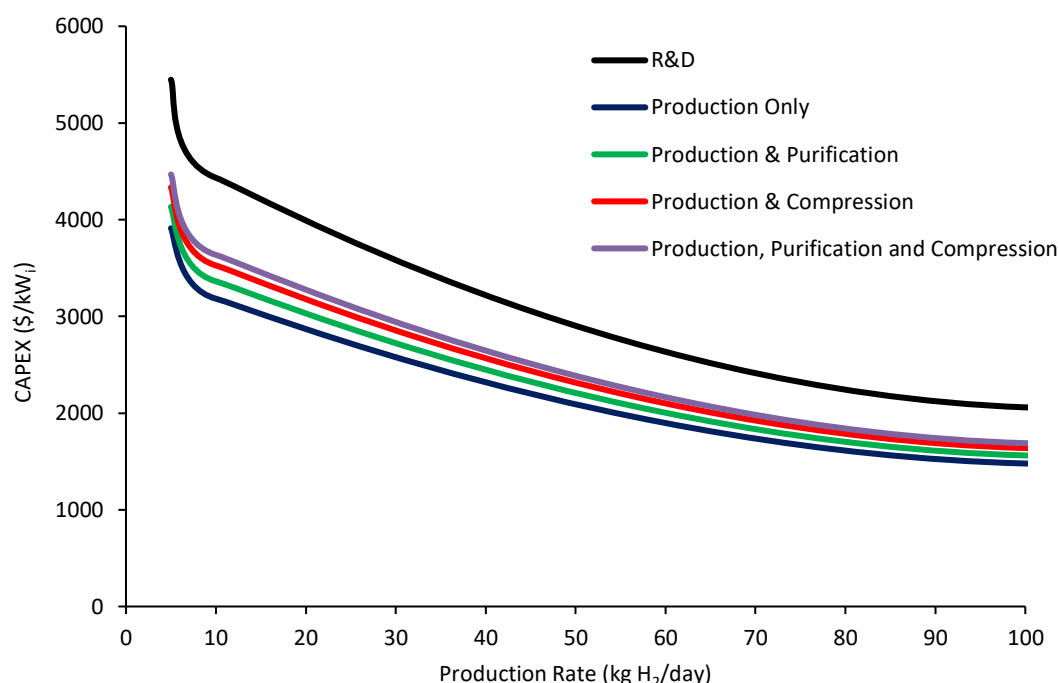


**Figure 6-3: The effect of scale up on CAPEX/kW<sub>installed</sub> for various configurations of the DEFT™ 2.5 unit - Values based on 80°C.**

As expected, the CAPEX of the system decreases with larger production rates. At 100 kg/day production, CAPEX values are predicted to be ~1 478.60 \$/kW<sub>i</sub>, which is below the expected 2000 \$/kW<sub>installed</sub>, as shown by Saur (63 HHV%) [18] and Hydrogenics (58 HHV%) [94]. At the industrial operating efficiency of 62.8 kWh/kg, a reduction of 21 % in CAPEX is achieved. At even larger scales of production, such as 1000 kg/day, CAPEX values are predicted to be approximately 686 \$/kW<sub>installed</sub> for a “Production Only” commercial unit, which is on par with industrial manufacturers as per the data provided in Figure 2-18 and Figure 2-21.

### 6.3.1.2 CAPEX Distribution of the DEFT™ 2.5 Unit

Figure 6-4 shows the cost contributions of the various components of the system CAPEX for a production only configuration. The CAPEX basis for this analysis was derived from the cost data applicable to the current DEFT™ 2.5 unit. This works off the cost data provided in Appendix E and includes the CAPEX savings listed in Table 6-3.

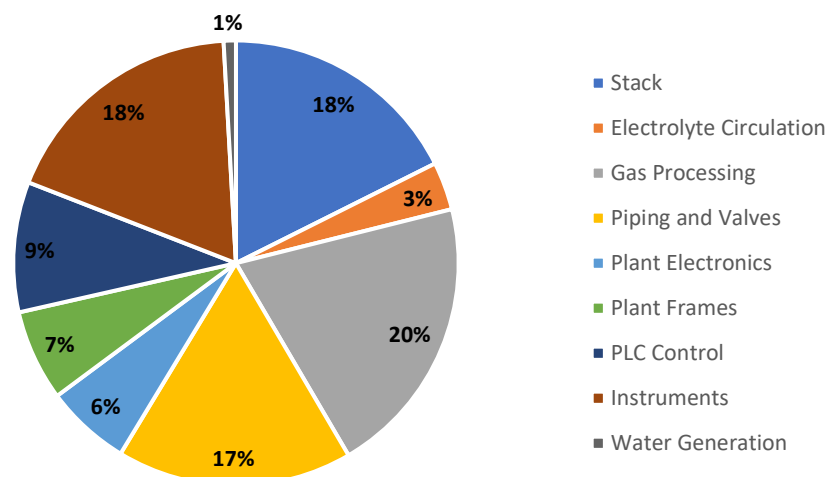


**Figure 6-4: Cost distribution of CAPEX for a 'Production Only' DEFT™ 2.5 unit.**

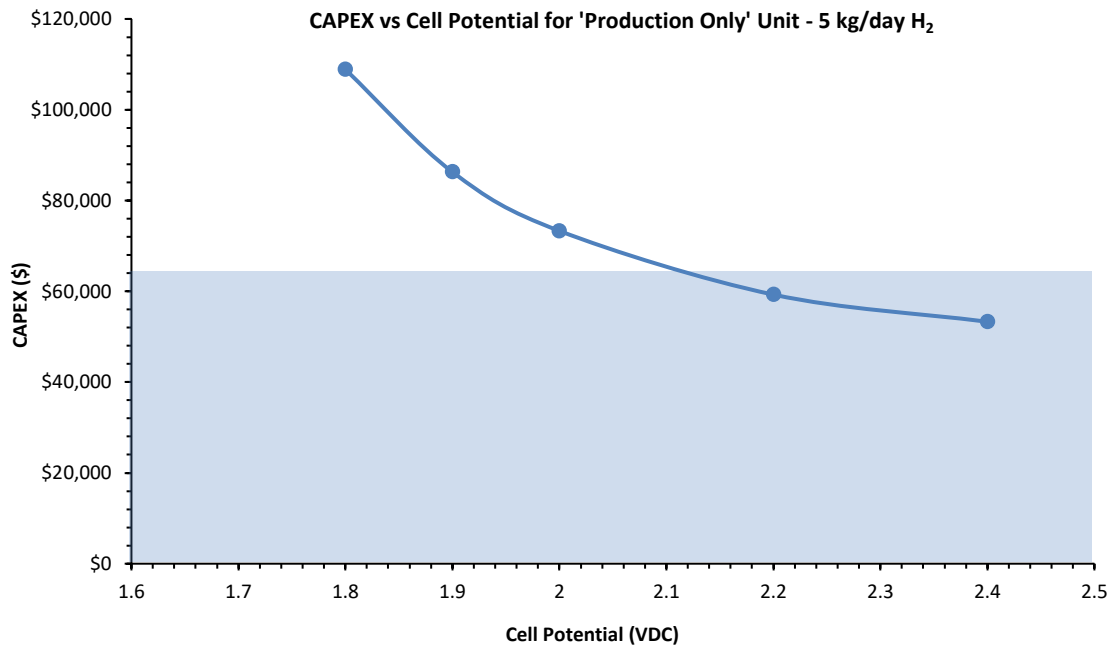
The electrolytic stack of the DEFT™ 2.5 system contributes approximately 18 % towards the total cost of the system. This is lower in comparison to conventional alkaline systems where the stack contributes between 30% of the total system CAPEX [93], [97]. This can be attributed to the stack not utilising a catalyst as of yet and the cost reduction associated with the absence of a conventional diaphragm/membrane. Furthermore, DEFT™ 2.5 electrodes are made from a simplistic nickel mesh that does not require any complex machining and pre-electrodes are not employed within this stack assembly. According to Ruth *et al.*, the use of a complex catalyst can represent approximately 6% of the total system costs, while conventional membranes account for approximately 3.5% of total costs [93], [95]. The cost contribution of gas processing is on par with that of industrial systems. Figure 2-21 shows that both small- and large-scale systems have a cost contribution of ~ 20% towards gas processing. Instrument costs are relatively higher than industrial standards, but this, however, will improve with scale.

#### **6.3.1.3 CAPEX of DEFT™ at Varying Operating Voltages.**

The current DEFT™ 2.5 unit does exhibit a significant reduction in CAPEX values when compared to market-related values, but this is achieved at a lower system efficiency. The unit does achieve the targets outlined in Section 1.2.2, but falls short of industrial standards for operating efficiency. The system was designed, however, to achieve the targeted production rates at a low system CAPEX (i.e. higher operating voltage). A sensitivity analysis was conducted on the operating voltages (indirectly the system efficiency) and the resultant system CAPEX. The system can be operated at lower cell potentials to reduce the electrical consumption of the stack, hence, allowing

for improved system efficiencies. The resultant production rate of hydrogen, however, is lower than the targeted 5 kg/day H<sub>2</sub> target. As such, the stack size of the current DEFT™ 2.5 unit would have been increased to allow for lower operating voltages/energy consumptions, which will ultimately increase CAPEX. The following results, provide in Figure 6-5, were obtained from the sensitivity analysis.

a)



b)

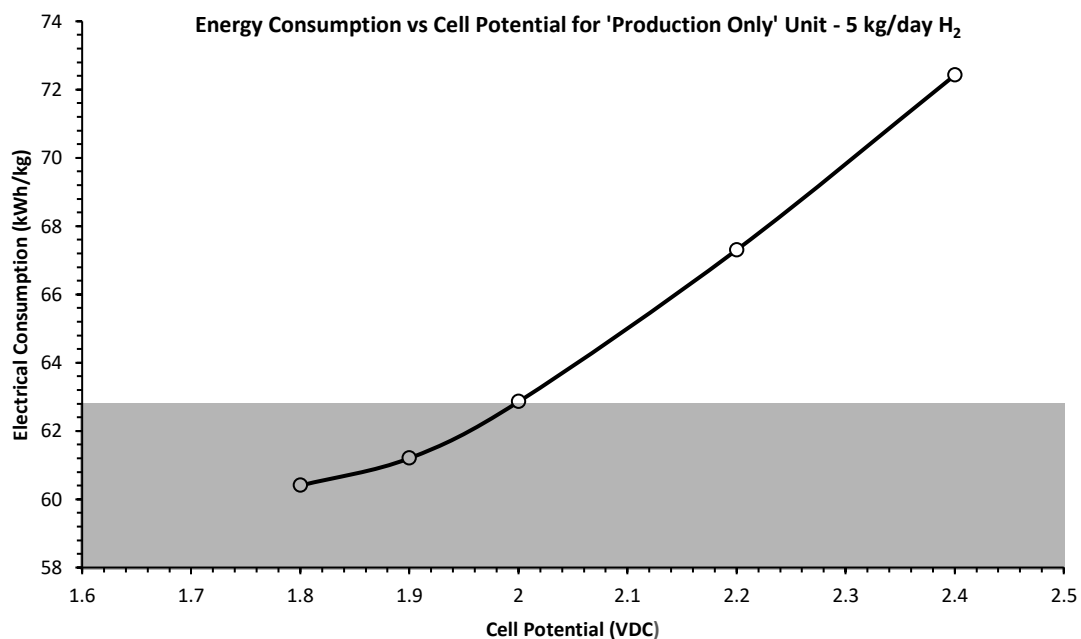
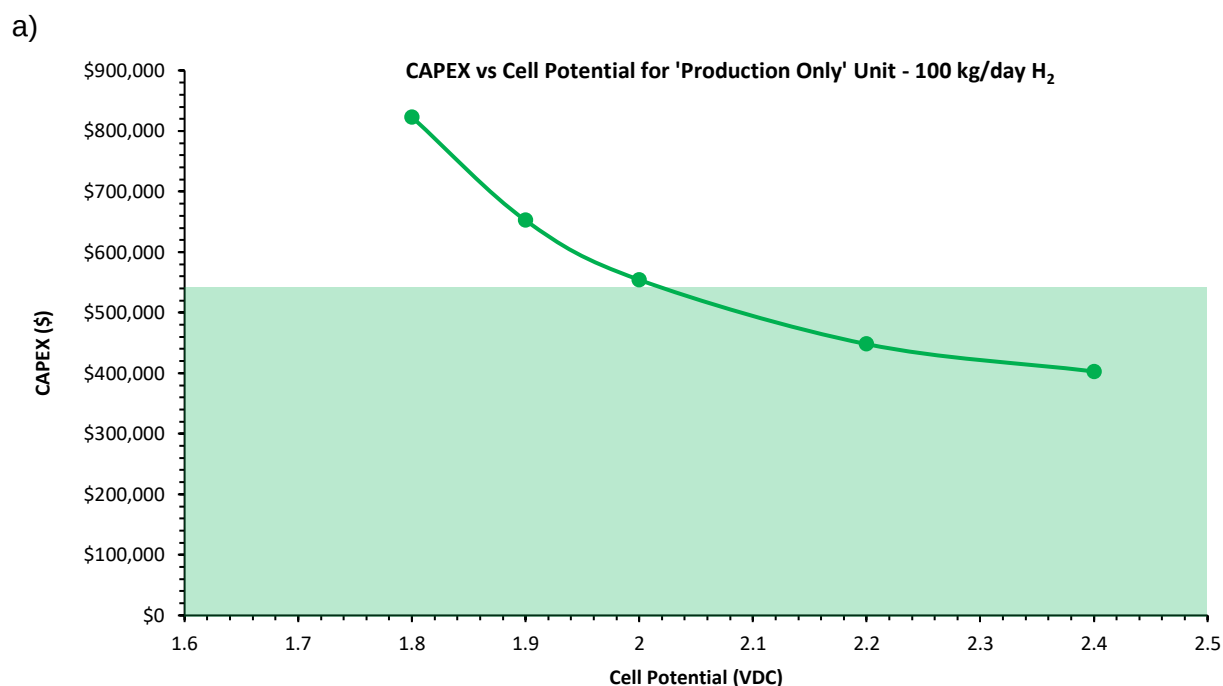


**Figure 6-5: a) Total CAPEX, b) Energy Consumption of a DEFT™ 2.5 'Production Only Unit' at varying cell voltages.**

Figure 6-5 shows the acceptable operating regions, according to Ivy [17] and Saur [18], for both system (a) CAPEX (blue region), and (b) energy consumption (grey region). The expected cost of a 5 – 10 kg H<sub>2</sub> alkaline electrolysis system, according to Saur [18], is \$65 000, while the expected energy consumption of electrolysis units are 62.8 kWh/kg H<sub>2</sub>. The blue and black line graphs represent the theoretical system CAPEX and energy consumption of a DEFT™ 2.5 unit, at varying cell potentials. A DEFT™ 2.5 unit falls within this region of acceptable system CAPEX at around 2.12 VDC, with a slightly improved energy consumption of ~ 65.2 kWh/kg H<sub>2</sub> (~ 2.83 % improvement from current operating energy consumption). Lowering the operating voltage to 2.12 VDC does not result in a low enough energy consumption to fall within the below 62.8 kWh/kg H<sub>2</sub> region. Operation below 62.8 kWh/kg H<sub>2</sub> can be achieved when the DEFT™ 2.5 unit is operated below 2 VDC, but the CAPEX of the system increases to roughly \$73 500 (5 852 \$/kW<sub>installed</sub>). therefore, the DEFT™ 2.5 unit cannot currently achieve both an acceptable CAPEX and energy efficiency without further cost and performance optimisation, but is rather suited to operate as either a 'Low CAPEX – High Energy Consumption' unit. To achieve this, further cost and/or performance optimisation of the current DEFT™ 2.5 unit must occur. The system would require a ~16.6% CAPEX (\$13 000) reduction at the current system performance operating at 2 VDC, or a ~ 4.9% (3.2 kWh/kg) improvement in system performance at the current system cost. This result will easily be achieved with the successful implementation of anodic and cathodic catalysts. The effect of economies of scale, with increased production capacities of 100 and 1000 kg/day H<sub>2</sub>, can be seen in Figure 6-6 and Figure 6-7:



b)

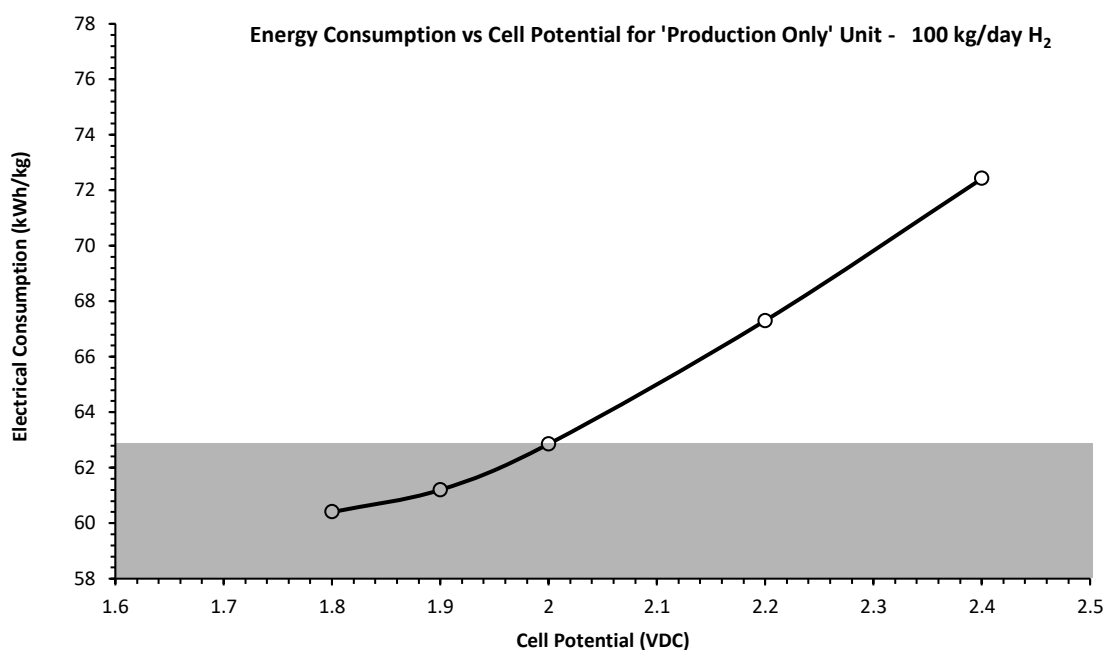
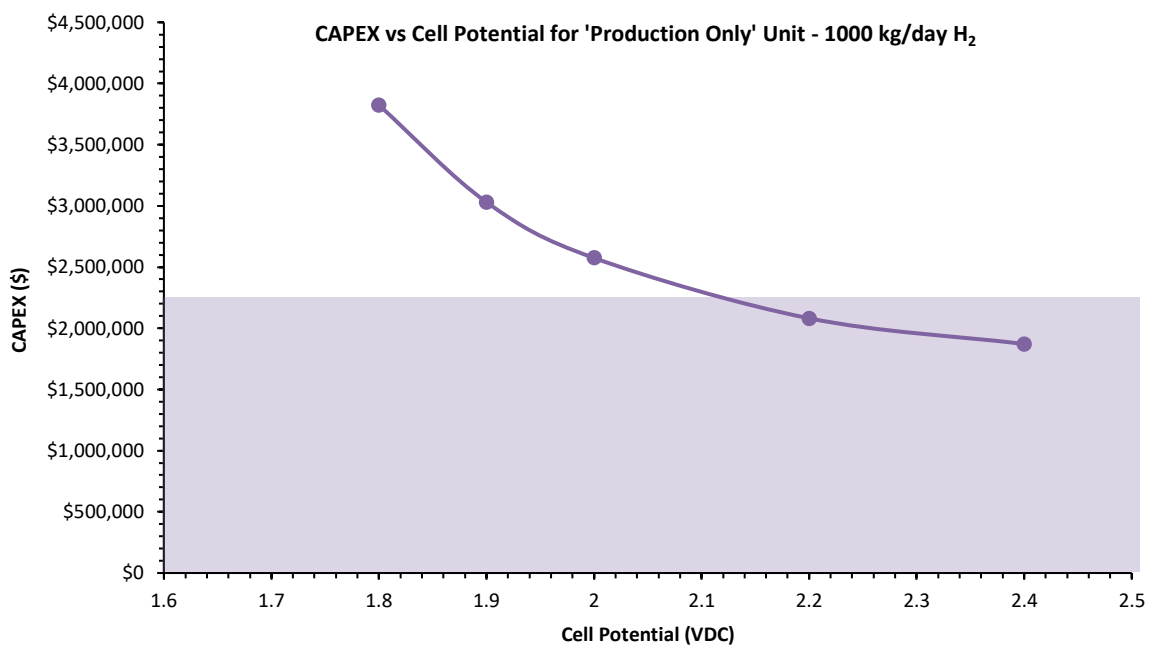


**Figure 6-6: a) CAPEX, b) Energy consumption of a DEFT™ 100 kg/day, 'Production Only' unit at varying cell voltages.**

a)



b)

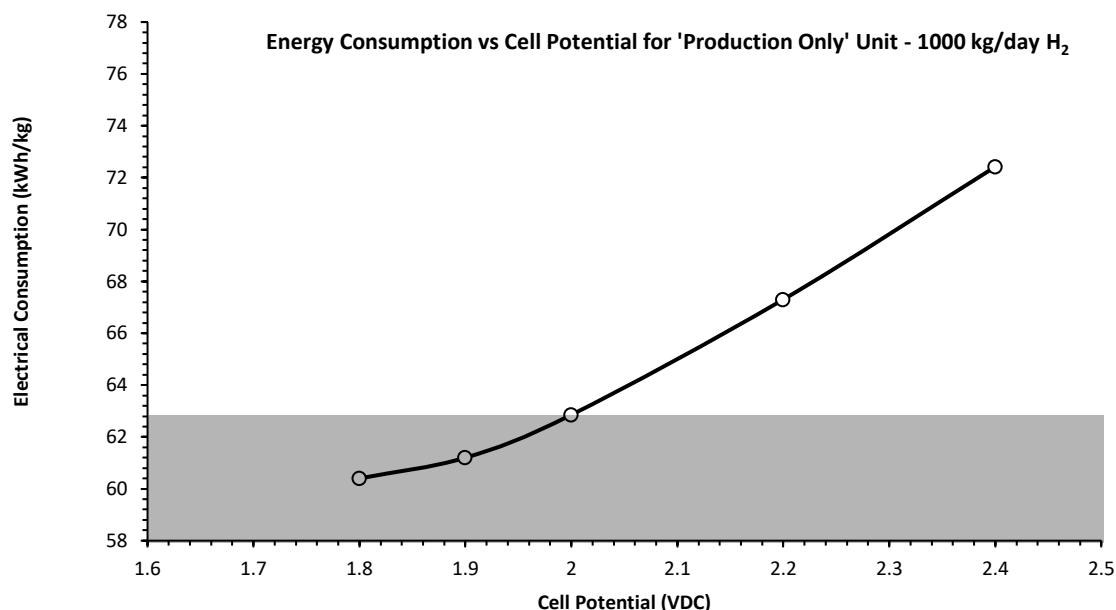


**Figure 6-7: a) CAPEX, b) Energy Consumption of a DEFT™ 1000 kg/day, 'Production Only' unit at varying cell voltage.**

Improvement in system CAPEX can be seen for the 100 kg/day production rate with the cost curve falling within the desired range at 2 VDC. At this operating point, the efficiencies curve enters the region of 62.8 kWh/kg H<sub>2</sub>. Although this operating point looks attractive it is only representative of a market entry point. State-of-the-art systems, such as what is provided by Hydrogenics (data provided in Table 2-10), achieve this CAPEX target of 2000 \$/kW<sub>installed</sub> at HHV efficiencies of 58% [94]. For a new technology to compete in this market an improvement of such would still be required.

At larger production rates of 1000 kg/day H<sub>2</sub>, acceptable system CAPEX is reached at higher cell potentials in comparison to the 100 kg/day production rates. The required CAPEX reduction is increased to 12.9% (~\$333 000), while the required energy consumption improvement is increased to 3.8% (2.5 kWh/kg). It is, however, noted that economics generated for a 1000 kg/day H<sub>2</sub> system, with a 5 kg/day H<sub>2</sub> plant as a basis may carry significant error, however, system CAPEX is expected to improve at these larger scales once a larger scale basis has been developed. The ability to scale is, however, held back by relatively low system performance. If cost and design optimisation were to occur after scale-up of the current DEFT™ design, a significantly high CAPEX investment would be required to carry out iterative design modifications and investigative work at large production scales. To avoid this, performance and cost optimisation must continue to be conducted at small scale first before scale-up can occur.

### 6.3.2 OPEX Data for the DEFT™ 2.5 Unit

The OPEX values for the DEFT™ 2.5 unit were calculated based on the maintenance and replacement costs of the plant. The system boundary considered when calculating the system OPEX includes maintenance and replacement for the entire system, including auxiliary systems. Electrical costs associated with the DEFT™ 2.5 unit were not included in the OPEX analysis, as electrical costs are the largest contributing factor to hydrogen production costs and will, therefore, be considered separately. Table 6-7 shows the breakdown of plant maintenance and replacements and the frequency at which they occur. Any equipment that is not listed is assumed to have maintenance cost that is insignificant over the lifespan of the plant.

**Table 6-7: Maintenance frequency and costs for the DEFT™ 2.5 unit.**

| Instrument                       | Maintenance Cost (\$) | Maintenance Frequency                                           | Total Maintenance Cost (\$) |
|----------------------------------|-----------------------|-----------------------------------------------------------------|-----------------------------|
| De-ionised Conductivity Sensor   | 164.60                | Replace every 5 years                                           | 493.81                      |
| Fixed Gas Detector               | 180.00                | Replace every 3 years                                           | 1 080.00                    |
| H <sub>2</sub> Gas Purity Sensor | 606.42                | Replace every 5 years                                           | 1 819.25                    |
| O <sub>2</sub> Gas Purity Sensor | 606.42                | Replace every 5 years                                           | 1 819.25                    |
| Electrolytic Pump                | 349.95                | 1 Replacement/Spare                                             | 349.95                      |
| Dosing Pump                      | 629.51                | 1 Replacement/Spare                                             | 629.51                      |
| Mesh Electrodes                  | 2 384.82              | Replace every 7 years                                           | 4 769.64                    |
| Reactor Gaskets                  | 920.31                | Replace every 7 years                                           | 1 840.63                    |
| Non-Conductive Layer             | 138.94                | Replace every 7 years                                           | 278.88                      |
| Moisture Filters                 | 82.00                 | Replace every 2 years                                           | 1 558.00                    |
| Uninterrupted Power Supply       | 35.71                 | Replace every 8 years                                           | 71.43                       |
| Piping Components                | 127.94                | Replace every 7 years                                           | 255.88                      |
| De-ionised Water Generator       | 308.00                | Replace yearly                                                  | 5 852.00                    |
| Gas purification plant           | 3 960.00              | Replace H <sub>2</sub> and O <sub>2</sub> sensors every 5 years | 11 880.00                   |
| Compressors                      | 296.27                | Replace yearly                                                  | 5 629.16                    |
| <b>Total OPEX costs (\$)</b>     |                       |                                                                 | <b>36 697.30</b>            |

The savings philosophy for the commercial configuration, as mentioned in the CAPEX analysis, is also applicable to the system OPEX. The following cost data, provided in Table 6-8, is obtained for the five different configurations of the DEFT™ 2.5 plant and is based on the operating conditions stated in Table 6-5.

**Table 6-8: OPEX cost data for various configurations of the DEFT™ 2.5 unit.**

| Configuration                          | Energy Load (kW) | OPEX (\$) | OPEX/kW <sub>installed</sub> (\$/kW) | OPEX/kg (\$/kg H <sub>2</sub> ) |
|----------------------------------------|------------------|-----------|--------------------------------------|---------------------------------|
| R&D                                    | 13.98            | 19 997.24 | 1 430.50                             | 0.55                            |
| Production Only                        | 13.98            | 19 997.24 | 1 430.50                             | 0.55                            |
| Production & Purification              | 17.1             | 31 877.24 | 1 863.71                             | 0.88                            |
| Production & Compression               | 15.23            | 25 626.39 | 1 682.72                             | 0.87                            |
| Production, Purification & Compression | 18.35            | 37 506.39 | 2 043.48                             | 0.85                            |

The OPEX for the DEFT™ 2.5 unit is approximately 37% of the total CAPEX cost for a 'Production Only' commercial unit. This, however, includes replacement and maintenance of the stack and all auxiliary equipment for the system throughout the plant's lifespan. Excluding stack, equipment, and instrumentation replacements, the remaining OPEX per year (this is taken over the 7-year lifespan of the stack) is approximately 3.4% of the system CAPEX. This is within the expected 2 - 5% presented by industry (data provided in Table 2-6). The system OPEX makes up 8.2% of the total lifespan system cost, which is marginally over the industrial standard of 8%. Included in the total lifespan system costs is the cost of electrical power supply. When calculating the total system costs, the cost of electricity was assumed to be 0.07 \$/kWh, obtained from a grid-solar combination system. OPEX contributions increase with the addition of purification and compression steps, as expected. According to Bertuccioli and Thomas, the estimated OPEX average for small neighbourhood sized alkaline systems is ~ 1500 – 1600 \$/kW<sub>i</sub> [93], [94]. At the industrial standard operating efficiency of 62.8 kWh/kg, this equates to a total system OPEX of \$19 521. The OPEX of the DEFT™ unit is therefore in line with industrial standards. The addition of gas purification and compression increase the OPEX percentage contribution to ~ 10% and 9.3% of the total system cost respectively, while the addition of both purification and compression steps increase the OPEX contribution to ~ 11%.

### 6.3.2.1 OPEX Distribution for the DEFT™ 2.5 Unit

Figure 6-8 shows the OPEX cost breakdown of the DEFT™ 2.5 unit, with the operating conditions mentioned in Table 6-5 set as the basis.

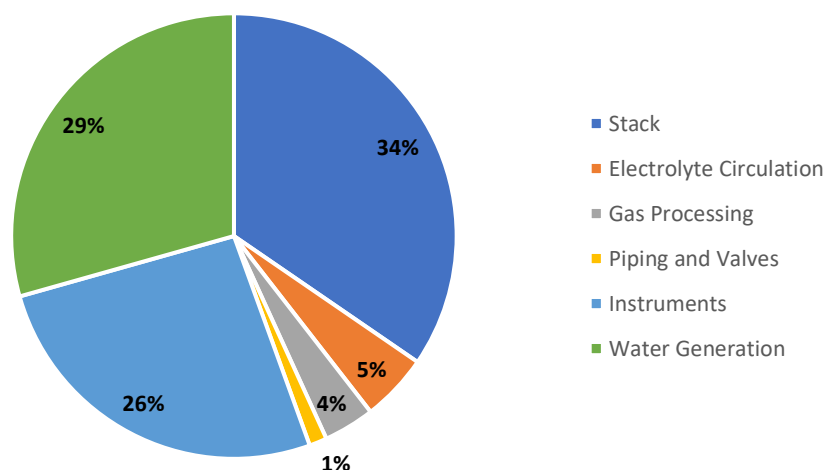


**Figure 6-8: Cost distribution of OPEX for the DEFT™ 2.5, 'Production Only' unit.**

The stack makes up the largest contribution towards the system OPEX, as stack replacement is included in this analysis. Water generation contributes significantly to the system OPEX, as the cation and anion-exchange resins require yearly replacement. The water generation maintenance costs could be the cause of the DEFT™ 2.5 OPEX being marginally higher than expected OPEX costs, however, this high cost for water preparation is in line with a small scale industrial system, as shown in Figure 2-21, where water preparation accounts for 35% of the BOP costs for a 10 kW system. Instrumentation costs also make up a significant part of the system OPEX accounting for 26% of the lifetime OPEX contributions. With scale-up, instrumentation and the cost of the water generation system would be offset with higher productions.

### 6.3.2.2 Economies of Scale for DEFT™ 2.5 OPEX

The effect of scale-up on the OPEX of the DEFT™ unit was investigated. Figure 6-9 shows the effect of economies of scale on the system OPEX. The scaling factors derived from the CAPEX analysis, shown in Section 6.2.3, were applied to the OPEX data for the DEFT™ system. The cost data provided in Figure 6-9 was based on the operating conditions of the DEFT™ 2.5 unit for all the mentioned configurations. The R&D curve is not visible in Figure 6-9, as it is overlapped

by the 'Production Only' curve. Both the R&D and 'Production Only' OPEX costs are of the same value.

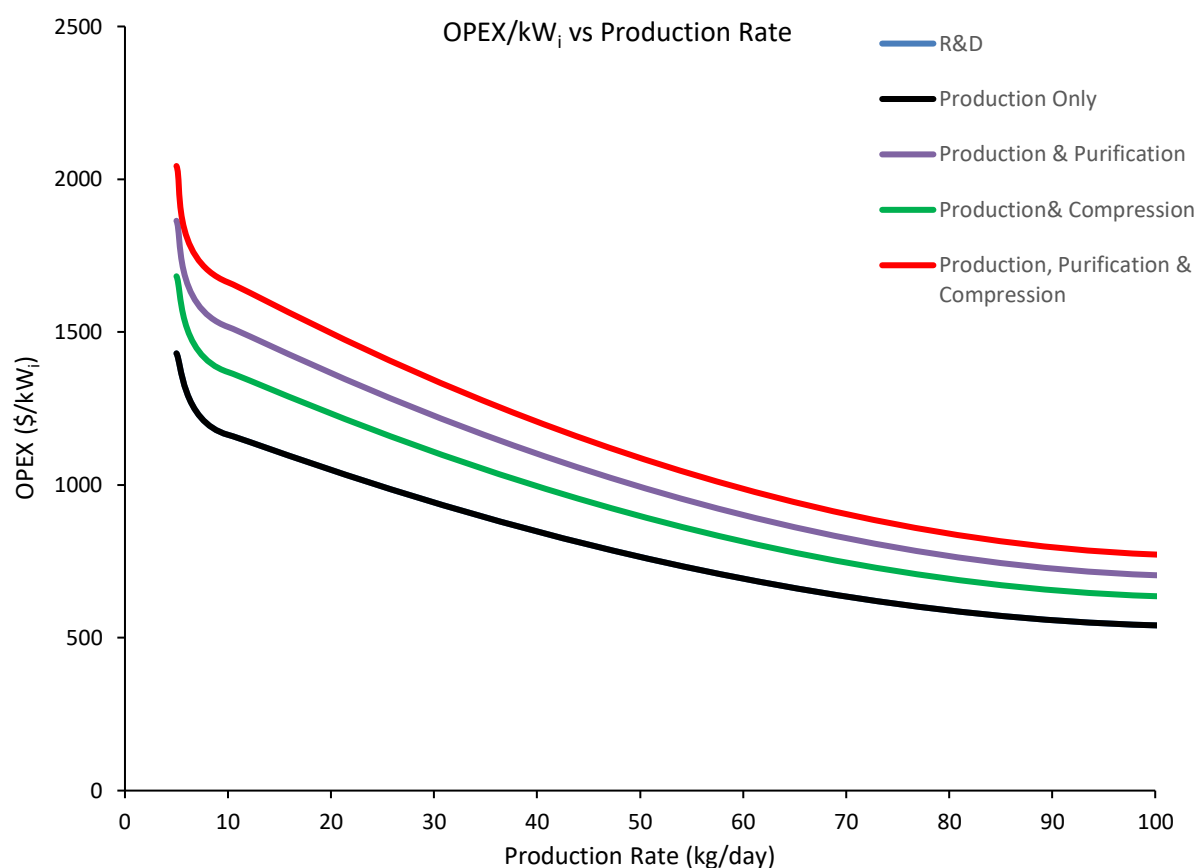


**Figure 6-9: Effect of scale up on system OPEX for the DEFT™ 2.5 unit for all system configurations.**

An expected decrease in OPEX with scale-up is observed in Figure 6-9. System OPEX has dropped significantly at production rates of 100 kg/day and above. At the 100 kg/day production rate, the percentage contribution of OPEX is ~ 4% of total system costs and at 1000 kg/day, this is further dropped to 2% of total system costs. The system OPEX still remains at 37% CAPEX for larger production rates, as the scaling factors used for this analysis are identical to that of the CAPEX analysis.

### 6.3.2.3 OPEX of DEFT™ at Varying Voltages

A sensitivity analysis on the OPEX of the DEFT™ 2.5 system was carried out to see the effect of varying operating voltages. Figure 6-10 shows the results of this investigation:

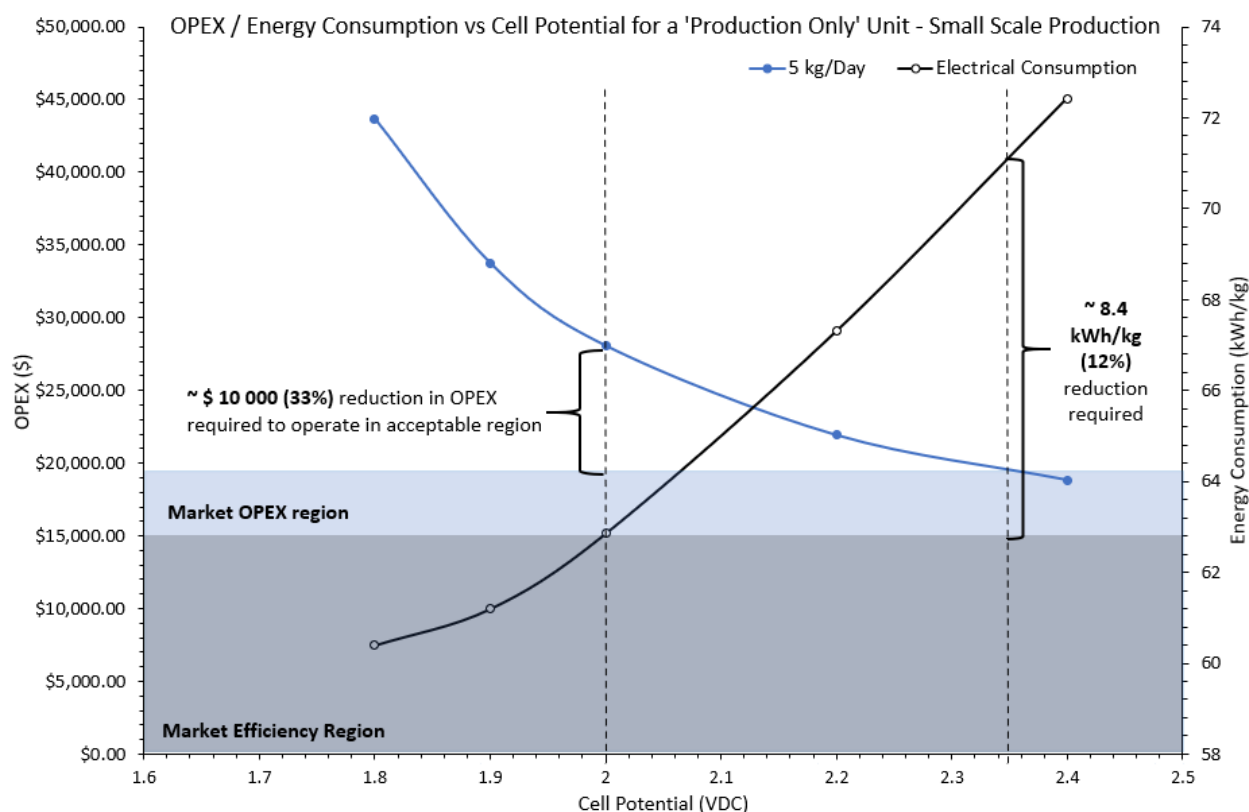


**Figure 6-10: OPEX/Energy consumption of the DEFT™ 2.5 'Production Only' unit at varying cell voltages.**

Again the “Market efficiency region” is defined at 62.8 kWh/kg H<sub>2</sub> and the “Market OPEX region” set at \$19 521. Similar to the CAPEX of the DEFT™ 2.5 unit, the system OPEX increases with decreasing cell potential. This is due to increased stack maintenance, as the stack size increases with lower cell potentials. OPEX values within the acceptable market region can be seen at  $\geq 2.3$  VDC. This cell voltage correlates with the current operating conditions of the DEFT™ 2.5 unit, as indicated in Table 6-5. The system OPEX is largely affected by the stack size. Reducing stack size through performance optimization would result in the largest OPEX reduction.

As noted, the efficiency curve enters the market efficiency region at 2 VDC. At this point, the overall lifespan OPEX cost is estimated at \$28 000. At this market efficiency entry point the lifespan OPEX cost needs to be reduced by \$8 500 - \$10 000 to show market competitiveness.

### 6.3.3 Hydrogen Cost Distributions for DEFT™ 2.5 Unit

Hydrogen production cost from electrolytic processes is primarily made up of system CAPEX, OPEX and electrical costs. The cost distributions for hydrogen produced from the DEFT™ 2.5 unit can be seen in Figure 6-11. The cost of electricity was based on a grid-solar combination system, with a price of 0.07 \$/kW, and an operating efficiency of 67.1 kWh/kg.

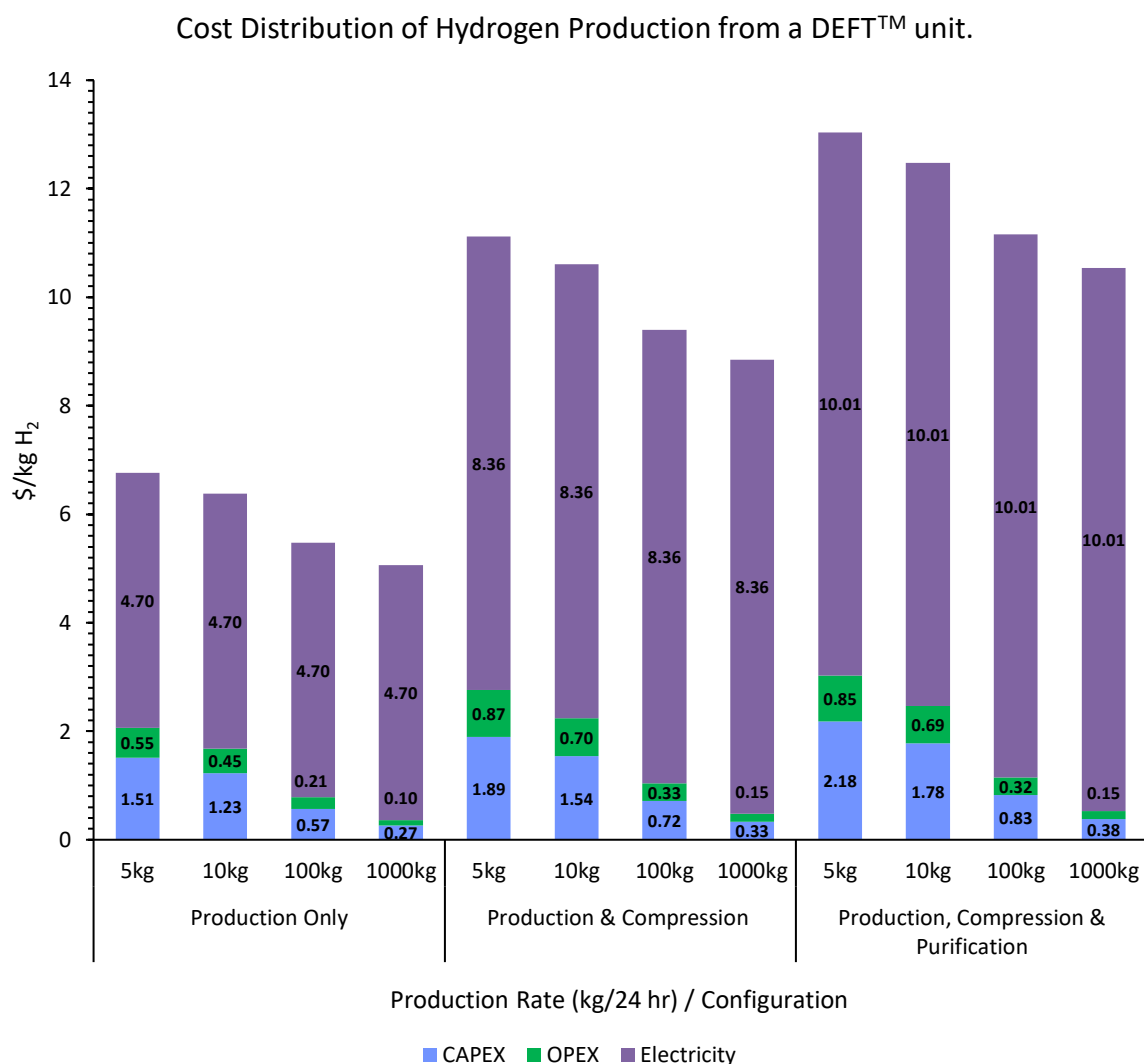


**Figure 6-11: Total cost contributions of CAPEX, OPEX and electrical expenses per kg H<sub>2</sub> for various scales and configurations of the DEFT™ unit.**

Figure 6-11 shows that the cost of hydrogen produced from a DEFT™ system ranges from 5.1 – 6.9 \$/kg for a ‘Production Only’ configuration. The \$/kg H<sub>2</sub> cost for a DEFT™ 2.5 unit falls within the expected industrial range of 5 – 7 \$/kg H<sub>2</sub> and is greatly improved with scale-up. The addition of purification and compression increases production costs significantly to > 8 \$/kg H<sub>2</sub>, missing

the industrial target of >\$7/kg H<sub>2</sub>. This implies that while the DEFT™ system is capable of reaching production costs close to the expected production costs of conventional electrolyzers, further cost optimisation must be implemented to achieve competitiveness within the hydrogen market. As stated, deployment of a catalyst and an increase in the active surface area of electrodes would work to reduce the overall electricity consumption as production rates could be achieved at voltages lower than 2.3 VDC. Figure 6-12 shows the percentage contribution of CAPEX, OPEX and electrical expenses towards the total production costs.

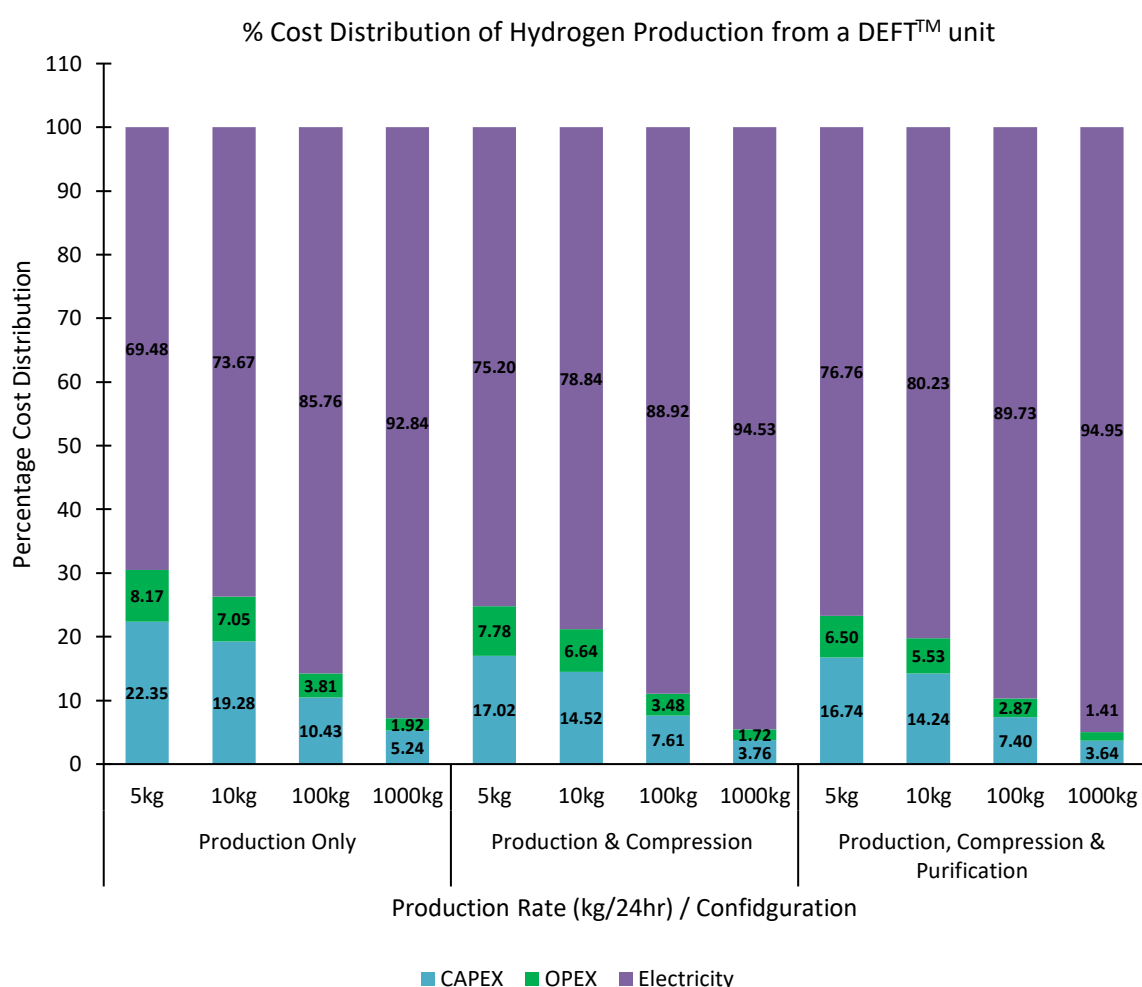


**Figure 6-12: Percentage cost contributions of CAPEX, OPEX and electrical expenses towards total hydrogen costs for various scales and configurations of DEFT™ unit.**

CAPEX contributions for the 'Production Only' configuration of the DEFT™ unit are ~7% lower than conventional systems and are further improved with scale. The same can be observed for the system OPEX. It is important to note that scale-up results in increased usage of electrical utility and works to offset the CAPEX contributions through greater production capacities, and as such, the electrical contribution towards system costs are increased. Electrical expenses are the

largest contributing factor towards the cost per kg of hydrogen, contributing ~ 69.5% of total costs for a 5kg 'Production Only unit'. Electrical expenses are expected to make up 50 – 70 % of total costs for conventional alkaline systems, according to the market analysis in Section 2.6.2 - Alkaline Water Electrolysis Techno-economics, places the DEFT™ 5 kg/day H<sub>2</sub> electrical consumption at the upper bound of the acceptable market range. Improving the electrical consumption of the DEFT™ unit would significantly lower the levelised cost of hydrogen. The electrical consumption of an electrolytic system is sensitive to factors such as the price of electricity and electrical efficiency of the unit. By sourcing low-cost electricity (renewable energy), and dropping cell potentials to achieve lower electrical consumption, hydrogen costs can be reduced significantly, making hydrogen produced by DEFT™ units more affordable and accessible.

#### **6.3.3.1 Sensitivity Analysis on Cost of Hydrogen and Voltage**

The effect of varying the cell potential on total production costs was investigated. In theory, dropping the cell voltage of the operating stack should lower the overall electrical consumption and, hence, decrease the associated cost to produce electrolytic hydrogen. This is noted as the electrical cost does carry the largest cost contribution. The reduction in cell voltage, however, works to increase the stack size consequently increasing CAPEX, hence, there exists a point where CAPEX vs OPEX play-off considerations need to be assessed. If no prior performance optimisation on the stack has occurred (i.e. current density remains the same at set voltage), the expected production capacity of the stack will decrease with lower operating cell potentials. To compensate for this, the stack size, as well as pumping requirements, must be increased. Figure 6-8 shows the resulting effect of varying cell potential on CAPEX, electrical and overall costs per kg hydrogen.

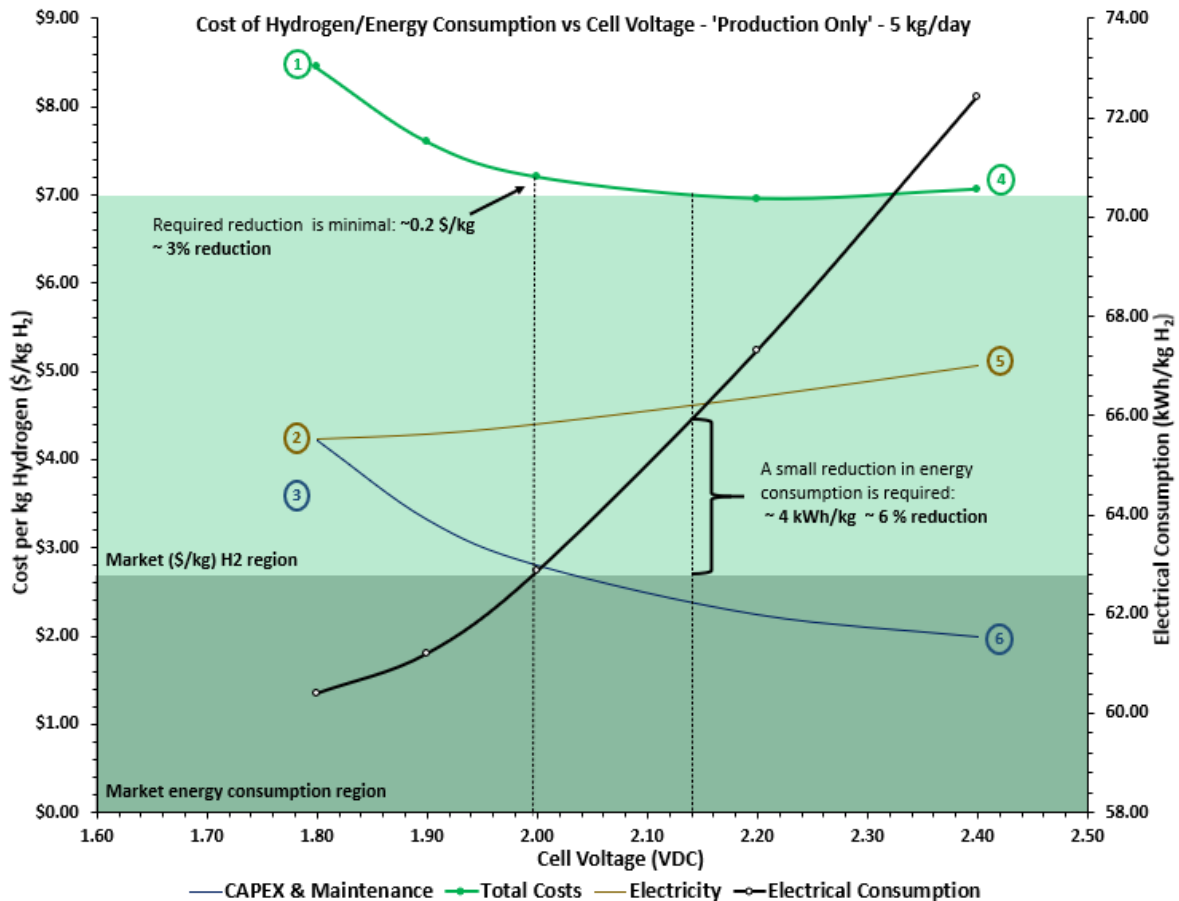


**Figure 6-13: Total cost per kg H<sub>2</sub>/energy consumption for the DEFT™ 2.5 'Production Only' unit at varying cell voltages.**

Figure 6-13 indicates the market viability of the DEFT™ 2.5 unit, and the minimum optimisation required to make the unit both cost effective and energy-efficient by industrial standards. The light green and dark green regions represent the acceptable cost region for hydrogen and the acceptable energy consumption region, respectively. It is observed that the cost of hydrogen curve for the DEFT™ 2.5 unit intersects the acceptable cost region between an operating voltage of 2.15 – 2.3 VDC, however, the electrical consumption at these conditions is higher than the market region. To obtain operation in both the cost and energy consumption regions, the cost of hydrogen for the system must be lowered by ~ 3 % (0.21 \$/kg H<sub>2</sub>), or the energy efficiency must be improved by 6% (4 kWh/kg). These improvements are, however, marginal. The DEFT™ 2.5 unit is operating close to the higher bound of the expected 5 - 7 \$/kg cost, while only making use of uncatalysed, standard, off the shelf, nickel electrodes. To this regard, DEFT™ has room for further optimisation to reach a production costs  $\leq$  5 \$/kg, and to increase market competitiveness. It is important to note that with the addition of an anodic and cathodic catalyst, as well as conductive supporting structures (pre-electrodes) the optimal voltage (lowest cost point) will shift to lower voltages with lower energy consumptions (higher efficiencies).

Furthermore, Figure 6-13 shows the respective effect of electrical cost and the combined effect of CAPEX and OPEX on the cost of hydrogen for the system. It is observed that both the CAPEX & OPEX and the electricity curve have varying effects on the total cost of hydrogen. At low operating voltages ( $\leq 1.8$  VDC), CAPEX & OPEX costs are at a maximum (Point 3) and result in the highest total cost of hydrogen (Point 1). Higher electrical expenses at higher operating voltages do increase total costs per kg hydrogen, but not to the extent of CAPEX & OPEX. This indicates that system CAPEX & OPEX dominate the cost of hydrogen for small scale production, and therefore produces the lowest \$/kg H<sub>2</sub> at efficiencies lower than current industry standards.

### 6.3.3.2 The Effect of Scale-Up on Total Hydrogen Costs

Scale-up of production capacity results in a significant improvement of the total hydrogen costs, with \$/kg H<sub>2</sub> values in the acceptable range for both consumption and cost per kg H<sub>2</sub>. The lowest costs per kg of H<sub>2</sub> are achieved at an operating voltage of 1.95 VDC as noted in Figure 6-14.

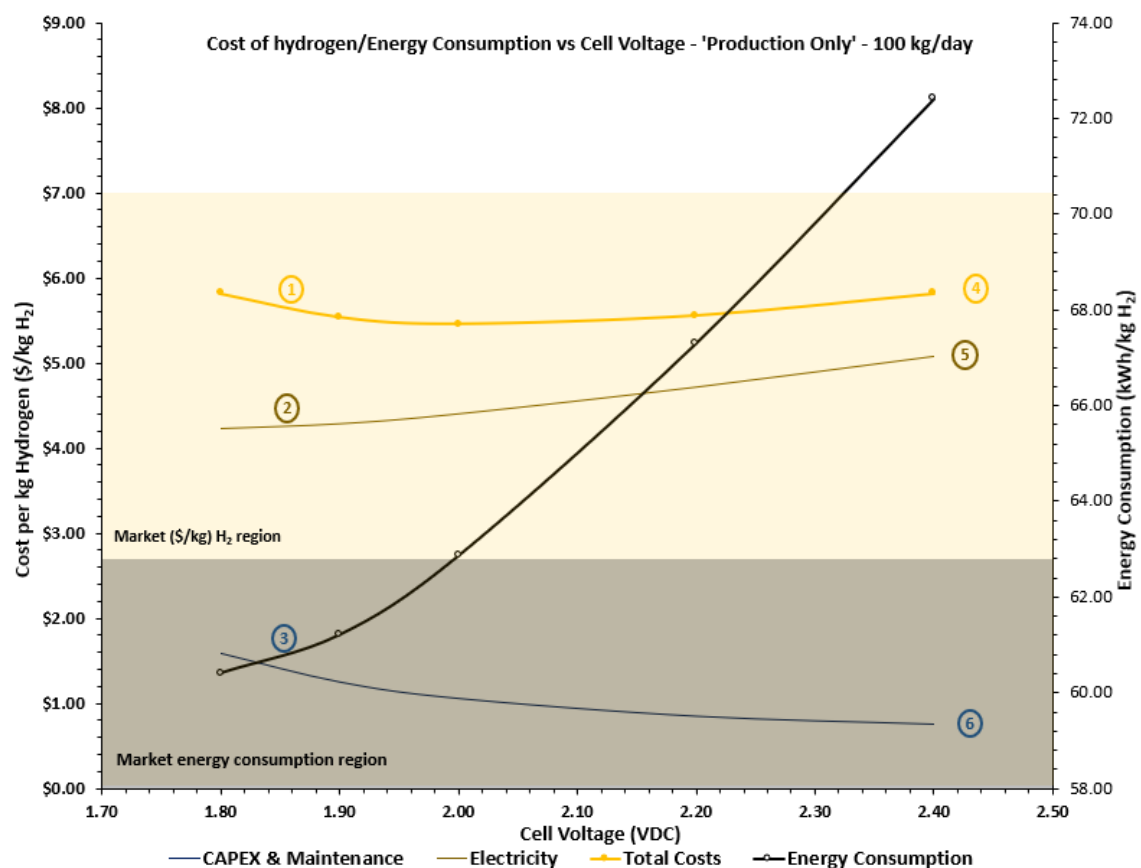


**Figure 6-14: Total cost per kg H<sub>2</sub>/energy consumption for the DEFT™ 100 kg/day 'Production Only' unit at varying cell voltages.**

Figure 6-14 shows that at greater hydrogen production capacity (in particular 100 kg/day H<sub>2</sub>) the cost of electricity has a greater effect on the total cost of hydrogen, in comparison to the 5 kg/day

H<sub>2</sub> unit. The highest \$/kg H<sub>2</sub> values are found at Points 1 and 4 of the curves, which correlates to the highest electrical and CAPEX & OPEX expense of the system. In contrast to smaller-scale units, CAPEX & OPEX contributions toward total costs decrease with larger production capacities. CAPEX per kg hydrogen is known to improve with scale, also contributing to the low CAPEX & OPEX cost per kg hydrogen observed in Figure 6-14 and Figure 6-15. It is therefore imperative that good electrical efficiencies are achieved with scaled production, as the weighting of electrical expenses towards total production costs increases with larger production rates.

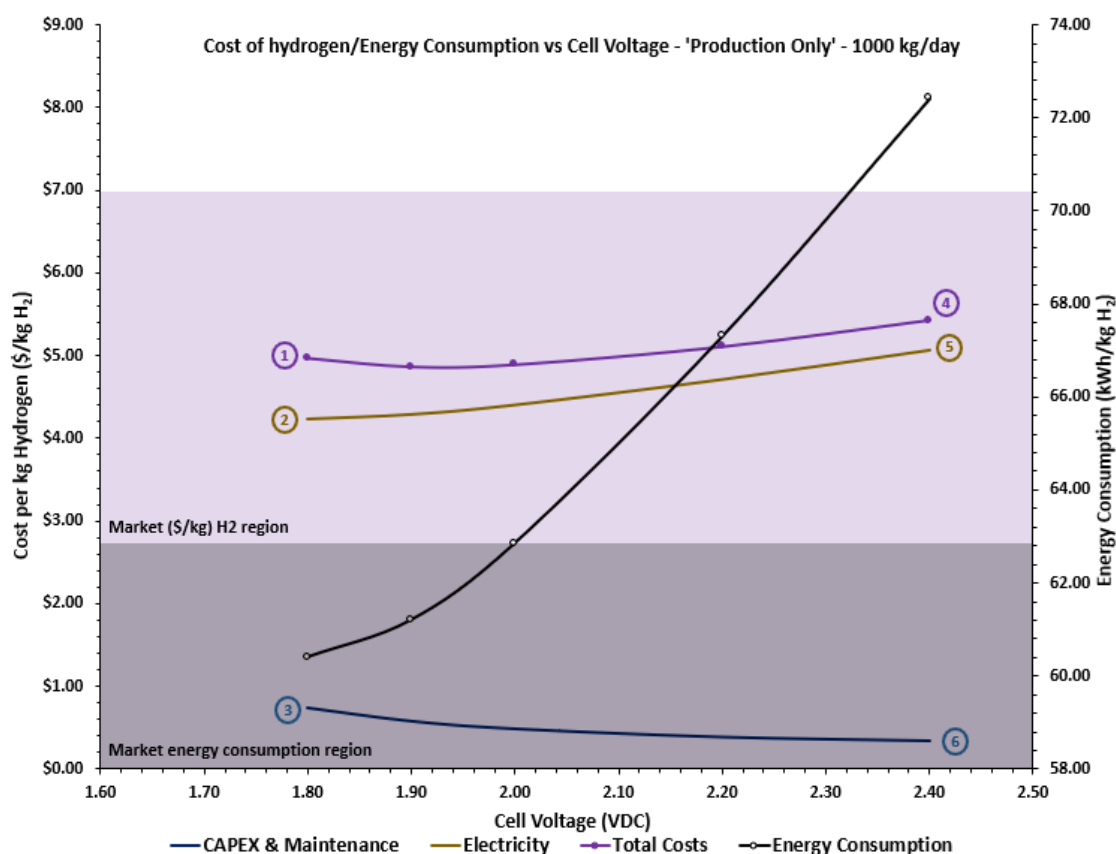


**Figure 6-15: Total cost per kg H<sub>2</sub>/energy consumption for the DEFT™ 1000 kg/day 'Production Only' unit at varying cell voltages.**

At 1000 kg/day production, the effect of scale-up lowers total hydrogen cost even further, with \$/kg H<sub>2</sub> values well within the acceptable market region. Electrical expenses dominate the overall cost of hydrogen, with curve 1-4 following an almost identical trend to that of curve 2-5. Hence the importance of optimising the technology before achieving scale-up.

### 6.3.3.3 The Effect of Electricity Price on Hydrogen Costs

With the electrical input costs carrying the highest weighting towards the overall cost to produce electrolytic hydrogen, changes in the cost per kWh of electrical input would consequently have a drastic effect on the presiding cost of electrolytic hydrogen. A sensitivity analysis investigating the effect of electrical input costs on production costs would provide benchmarks for which electrolytic hydrogen production can be deemed cost-effective or intensive. The curves are provided for “Production Only”. Additional curves for other configurations are provided in Appendix F.

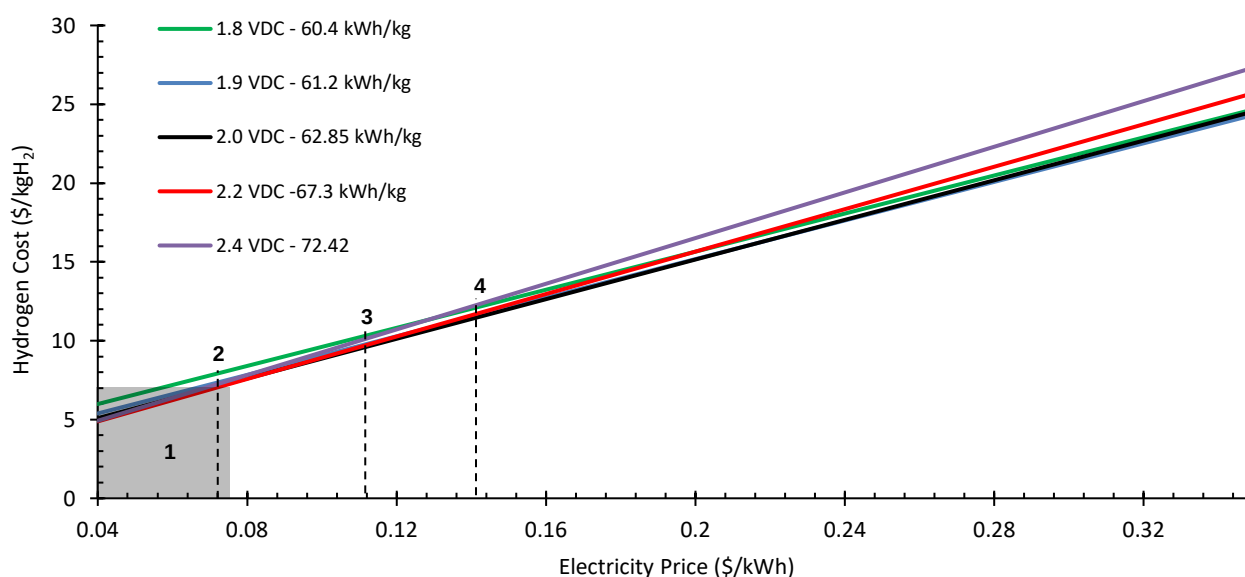


**Figure 6-16: Hydrogen Cost per kg versus electricity prices for a DEFT™ 2.5 ‘Production Only’ unit.**

It is observed in Figure 6-16 that high voltage operation results in the highest hydrogen cost with increasing electricity prices. This can be expected, as the 2.4 VDC operation correlates to the lowest energy efficiency, resulting in the highest energy consumption for a 5 kg/day production rate. The inverse can be seen for low voltage operation, where hydrogen costs are the highest at low electricity prices, due to relatively high CAPEX costs, and the lowest at high electricity costs. Point 1 in Figure 6-16 indicates the region of 5 – 7 \$/kg H<sub>2</sub>, which has been determined as the industrial benchmark for hydrogen production costs. In its current unoptimised form the DEFT™ 2.5 unit can operate in this region at electricity prices of < 0.04 – 0.08 \$/kWh. Point 2 on Figure 6-16 shows an electricity price of ~0.07 \$/kWh from a grid-solar combination source. Point 3 shows an electricity price of 0.11 \$/kWh from a South-African service provider, while point 4 shows the average electricity price of 0.14 \$/kWh from a US service provider, further electrical prices can be extracted from Table 2-8. In its current form, DEFT™ units are competitive at electricity prices < 0.08 \$/kWh which can be achieved by renewable energy sources, yet,

renewable energy sources, in particular solar, are incapable of providing electricity at all times of the day (intermittent). This low capacity factor negatively affects production economics therefore it is recommended that these systems be tied to grid electricity. Electricity sourced from the grid would prove to be unfeasible at this scale in many countries, including South Africa, due to the relatively high electrical costs. At higher production rates, hydrogen costs are expected to drop significantly, allowing for more flexible operation in terms of electricity prices.

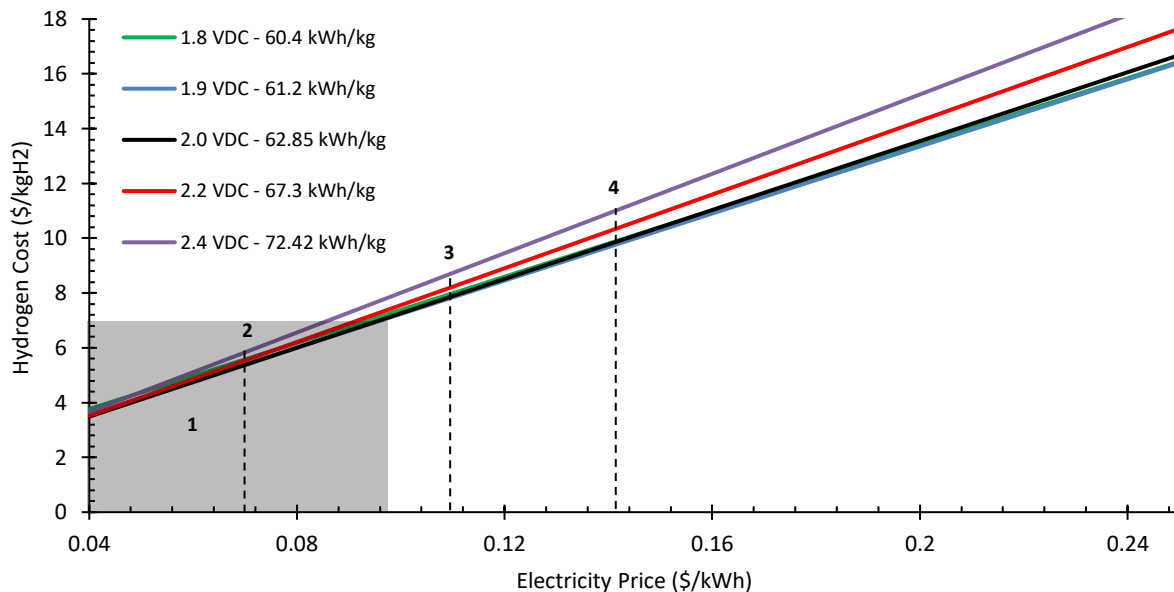


**Figure 6-17: Hydrogen costs versus electricity prices for a DEFT™ 100 kg/day 'Production Only' unit.**

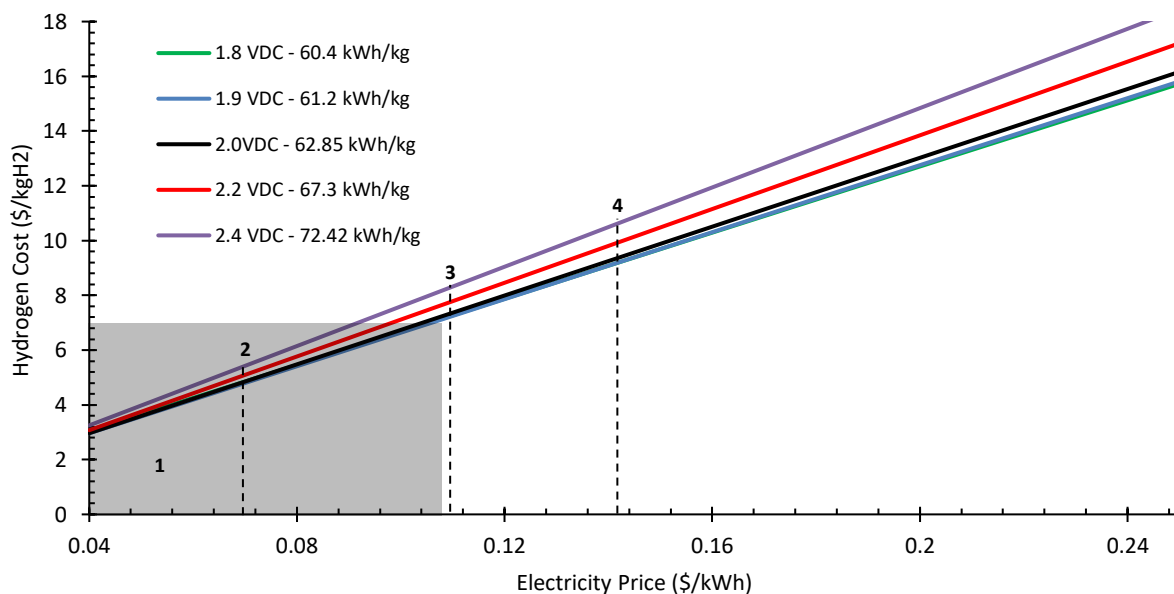


**Figure 6-18: Hydrogen costs versus electricity prices for a DEFT™ 1000 kg/day 'Production Only' unit.**

From Figure 6-17 and Figure 6-18, scale-up has resulted in region 1 expanding over slightly higher electricity prices. This indicates that a DEFT™ 100 and 1000 kg/day unit would be capable of fulfilling the 5 - 7 \$/kg H<sub>2</sub> requirement at higher electricity prices of 0.104 and 0.108 \$/kWh respectively. The ideal operation of DEFT™ units would, however, use low-cost renewable energy sources as an electrical feedstock to the system, balanced by a grid supply to supplement continuous operation.

## 6.4 Conclusions

The DEFT™ 2.5 unit was designed and manufactured as part of Phase 3 of the project. The unit was intended to be a proof of concept for the DEFT™ technology in the small neighbourhood production scale and was required to meet the specific objectives listed in Section 1.2.2. A techno-economic analysis was conducted to determine whether the project objectives were met by the DEFT™ 2.5 unit. Table 26 summarises the findings of this analysis:

**Table 6-9: Comparison of project objectives and DEFT™ 2.5 operating parameters.**

| Project Objectives                                                                                                                                                        | DEFT™ 2.5 Unit Outcome                                                                     |
|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| An overall system energy consumption of <b>&lt;90 kWh/kg H<sub>2</sub></b> – includes all auxiliary systems                                                               | 67 kWh/kg                                                                                  |
| Hydrogen costs <b>&lt; 7.5 \$/kg H<sub>2</sub></b> , with the CAPEX of DEFT™ units <b>&lt; 5 \$/kg H<sub>2</sub></b> for small scale production ( <b>&lt;20 kg/day</b> ). | Hydrogen Cost: ~ <b>6.76 \$/kg H<sub>2</sub></b><br>CAPEX: <b>1.51 \$/kg H<sub>2</sub></b> |
| Efficient gas/liquid separation with hydrogen and oxygen gas purities <b>&gt; 99 Vol%</b> .                                                                               | H <sub>2</sub> Gas purity: <b>98.9 - 99.23 Vol%</b>                                        |
| The unit must demonstrate feasible scale-up (3 – 5 kg/day) from laboratory scale.                                                                                         | 5 kg/24 hr production rate achieved.                                                       |
| Parasitic loads <b>&lt; 35%</b> of total power consumption.                                                                                                               | Parasitic load lowered to <b>3-8 %</b> of total energy consumption.                        |
| The unit must demonstrate long term stability                                                                                                                             | *1000 hr test on the unit has been completed.                                              |

From the techno-economic analysis, it was found that the total hydrogen production costs of the unoptimised DEFT™ 2.5 unit were found to be between 6.7 – 9 \$/kg H<sub>2</sub> for electricity prices varying between 0.07 – 0.11 \$/kWh. System CAPEX was found to 1.51 \$/kg H<sub>2</sub>, which is relatively lower than the industrial standard. This equates to an ~ 21% reduction in CAPEX, in comparison to current small-scale electrolyser in the market. The system OPEX for the DEFT™ 2.5 unit was found to be ~ 0.55 \$/kg, which is on par with industrial standards. The initial design of the DEFT™

2.5 unit targeted a 5 kg/day H<sub>2</sub> production rate at a relatively low system CAPEX. Upon testing of the DEFT™ 2.5 unit, it was found that the above production target was met, but at energy consumptions higher than industrial standards. While the energy consumption of 67 kWh/kg H<sub>2</sub> does fulfil the >90 kWh/kg H<sub>2</sub> requirement, it does not satisfy the requirements for a competitive electrolysis system within industry.

A sensitivity analysis was conducted by varying the cell potential of the electrolytic stack, in an attempt to achieve improved energy efficiencies. It was found that to maintain the targeted 5 kg/day H<sub>2</sub> production rate at lower operating voltages, the stack size of the system needed to be adjusted accordingly, resulting in an increased system CAPEX. While efficiencies incrementally improved at cell voltages  $\leq 2.2$  VDC, the resultant system CAPEX was found to be higher than industrial standards. An operating point exhibiting both low CAPEX and good operating efficiencies could not be found for the current unoptimised DEFT™ 2.5 unit, due to a lack of cost or performance optimisation. This result is, however, expected for an unoptimised system using off the shelf, standard nickel electrodes. Scale-up of the DEFT™ 2.5 unit to larger production sizes does provide an improvement to both the CAPEX of the unit and the overall production costs of hydrogen. While the current design of DEFT™ 2.5 does satisfy all the objectives of the listed in Section 1.2.2, the electrode assembly must be optimised to successfully penetrate the hydrogen market. This can be successfully achieved by employing the correct catalysts to the electrode assembly and further modification of the electrode configuration/assembly.

## CHAPTER 7 - RESEARCH CONCLUSIONS AND FUTURE WORK

### 7.1 Conclusions

The purpose of this study was to address the parasitic load and flow path limitations associated with an earlier demonstration plant of the DEFT™ technology. In doing so a system that exhibited higher system efficiencies and the ability to scale would potentially result. With design modifications carried out to the electrodes' design, the electrolyte injection manifold, the stacks' power distribution philosophy and with the incorporation of a non-conductive mesh to target improved flux distribution, the DEFT™ technology was capable of producing hydrogen gas at purities > 99 vol% at flow velocities as low as 0.0004 m.s<sup>-1</sup>. This notes a substantial reduction compared to the originally specified flow velocity of 0.075 m.s<sup>-1</sup>. This resulted in the system achieving commercial benchmarks with regard to rated system efficiencies and CAPEX.

While the DEFT™ 2.5 system was able to meet the objectives of the project, listed in Section 1.2.2, the performance of the system, in its unoptimised state, still does not competitively compare to current state-of-the-art alkaline systems. With further development, by targeting operating conditions that would not be possible with the operation of conventional diaphragm units, the DEFT™ technology could become competitive within the hydrogen market. However, the following performance issues with the system must be addressed first:

#### **1. No noticeable benefit in current densities and system efficiencies.**

The DEFT™ 2.5 system was operated at electrolytic flows between 10 – 45 L.min<sup>-1</sup>, in an attempt to reduce the parasitic load of the system, while still gaining the benefit of reducing bubble coverage, and subsequently improving current density. At these flow velocities, the current densities achieved by the DEFT™ system showed minimal observable benefits in comparison to conventional systems, with system energy consumptions still being > 60 kWh/kg H<sub>2</sub>.

In the realm of the low electrolytic flow design, little benefit to the performance of the cell was noted while operating at higher electrolytic flow rates (compared to conventional technologies). Although the incorporation of catalysts would benefit the DEFT™ technology's performance and production economics, the same benefit would be exhibited in a conventional diaphragm cell. In like for like comparisons, provided in Section 5.4.4, the DEFT™ technology exhibited performance whereby a slight improvement was noted over a conventional zero-gap configuration. For a new technology, incorporating a novel operating principle, it would need to show a substantial benefit over existing technologies. In the current state of the DEFT™ technology, this advantage has not

yet been experienced. The technology, however, is in a state of close comparison to conventional technology with the potential to push the boundaries of conventional technologies. At the reduced flows, the technology still has the potential to make use of the flow-through principle in conjunction with electrodes of high density to target flow-assisted performance boosts, a principle which is unachievable through conventional diaphragm cells. It is, therefore, concluded that the DEFT™ technology does not show performance benefits operating in the realm of conventional electrolyzers i.e. standard mesh electrodes, at conventional temperatures, conventional pressures, and conventional electrolyte specifications. In other words, the DEFT™ technology operating at standard conditions, at comparable system efficiencies, does not result in a substantial reduction in cell resistances. The added benefit of better bubble management and increased specific conductivity is subsequently minimised due to the presence of a larger electrode gap and increased parasitic loads (when compared to conventional systems).

## **2. Higher electrolytic flows are still required to obtain an adequate gas separation.**

Relatively high flowrates are still required to maintain safe gas separation within the stack. At the lower end of the chosen electrolytic flowrate range, gas separation at higher operating temperatures is still not adequate, with oxygen being produced at purities approaching the explosive range (hydrogen in oxygen LEL). Furthermore, an observable volume of purge gas is still produced within the system, indicating inadequate separation. This could be improved by using alternative materials for the non-conductive separator and introduction of materials with low gas permeability will improve product gas separation at low electrolytic flowrates, but may have an adverse effect on ohmic resistances of the system.

Although the parasitic load associated with pumping has reduced drastically, now accounting for roughly 3 – 8% of the total power consumption, the flow is still considerably high that presents challenges in scale-up and works to hamper market penetration. Operating at 45 L.min<sup>-1</sup> and assuming operation at 2 VDC, according to the data provided in Section 5.4.3, would result in a current density of 200 mA.cm<sup>-2</sup> and a daily production rate of 3.4 kg/day H<sub>2</sub> from the electrode area installed in the DEFT™ 2.5 unit. Assuming extension to a 100 kg/day H<sub>2</sub> plant (250 kW), a total solution flowrate of 1 324 l/min would be required to maintain the same flow velocity (0.0004 m.s<sup>-1</sup>). The circulation, make-up, handing, storage, and later disposal of such a large volume of corrosive liquid is undesirable.

### **3. Flow path limitations**

A nylon mesh was introduced into the Bipolar Bi-MCFP stack to target uniform flow distribution across the electrodes. Despite this addition, the flow path of the electrolyte remained limited, preventing the scale-up of the technology to appreciable unit sizes. The flux distribution across the electrode is dependant of the aperture rating of the non-conductive mesh. For scale-up multiple injection ports may be included in the electrolyser's design, which would provide a large cell structure while the flow path limitation is adhered to.

For greater flow paths smaller aperture ratings (lower porosity) for the non-conductive layer would be required, however, smaller aperture ratings work to increase cell resistances and increase the pressure head requirement. Further to this, if the technology works to reduce the flow entirely through aperture restriction of the non-conductive mesh then the DEFT™ technology would start to emulate that of a conventional electrolyser. The operating principle of the DEFT™ must remain reliant on flow-based separation as this results in a mechanical means of maintaining separation, therefore, the technology will keep its flexibility and versatility intact that allows it to easily adapt to a variety of applications. In summary, the technology must be developed such that it works to push the boundaries of conventional electrolysers as opposed to trying to compete with conventional electrolysers within the realms of the same operating conditions. The technology, therefore, needs to be developed such that it truly exploits its membraneless operating state.

## **7.2 Future Work and Recommendations**

The current DEFT™ 2.5 unit, with further optimisation of the design, can be applied to some niche applications within the hydrogen market. These include:

- 1) sustainable storage solutions for curtailed renewable systems,
- 2) back-up energy and micro-grid applications, and
- 3) small scale applications in the hydrogen market (Please refer to Figure 10 in the market analysis section).

To produce a fully commercialised unit that applies to the broader hydrogen market, the DEFT™ unit must be capable of feasible scale-up to large productions, while maintaining efficient and safe operation. To achieve this, further development of the current DEFT™ design would be required. While the performance of DEFT™ in its current state may not show a significant benefit over conventional electrolysis systems, the technology still has the potential to address specific, niche applications within the hydrogen market.

### **7.2.1 High Current Density Operation.**

DEFT™ units can potentially aid in the balancing of grids that are powered by renewable energy technologies (curtailed energy utilisation). This would require electrolysis units to be capable of handling high current density operation and fluctuating loads, due to high peaks in energy production at low demand periods. The presence of high electrolytic flow within the system allows for effective handling of heat and the reduction of heightened bubble coverage, as well as reducing the potentially high ohmic resistances in the electrode gap, which increase the system's capability to handle high current densities.

Furthermore, the DEFT™ technology can be improved to achieve high current densities through the employment of dense electrodes with high surface areas. Conventional systems are not able to make use of high surface area electrodes due to the mass transfer limitations associated with them. This is, however, mitigated by the increased diverging flow provided by DEFT™ units. It is important to note that high parasitic loads will be associated with the above-mentioned operation, and as such, the electrical consumption associated with this DEFT™ system will most likely be substantially higher than current electrolysis technologies. If the optimal relationship between electrode configuration and electrolytic flow is developed, such that the benefits from increased current densities significantly outweigh the high parasitic loads, it is a possibility that DEFT™ can provide a solution to high current density operation applications at reasonable energy efficiencies, providing a low CAPEX system in a scenario where OPEX contributions are not the preceding cost factor.

### **7.2.2 Electrolysis of Impure Water Sources – Urea, Saltwater, Acid-mine drainage**

Several companies and institutions have approached Hydrox Holdings Ltd. with the intention of applying the DEFT™ technology for the electrolysis of contaminated water. A common problem faced with the electrolysis of impure water is the degradation/fouling of the membrane within the electrode assembly of the unit. The DEFT™ operating principle addresses this issue through the operational flexibility of the plant, as well as the absence of a conventional/diaphragm. Additional complexities include low conductivities of the associated electrolytes and the presence of contaminants and particulates that would result in sludge build-up in the cell. However, the DEFT™ operating principle provides a versatile basis to assess operating the electrolyser with unconventional feedstocks.

### **7.2.3 Intermittent Loads – Linkage to Renewable Energy.**

A further problem faced by the green hydrogen market is possible operational complications associated with the linkage of conventional electrolyzers to renewable energy. Conventional electrolysis units operating off intermittent loads may result in membrane rupture and often suffer from poor gas purities (high H<sub>2</sub>O transfer) at partial loads due to low power periods. Furthermore, each component of a conventional system is designed around specific conditions and parameters, making the system sensitive to fluctuations in the plant conditions. Due to the flexibility of the DEFT™ design, and the absence of a conventional membrane/diaphragm, sensitivity to fluctuations in the power load can be significantly reduced.

### **7.2.4 Medium Temperature Operation.**

Conventional electrolyzers currently waste ~ 30% - 40% of the electrical feed as waste heat as these systems are limited to an operating temperature of < 90°C. Electrolysis systems with operating temperatures between 150 – 300°C can achieve a 30% reduction in electrical demand of the stack, due to the substantial drop in the electrical demand with increasing temperature. Further to this, this temperature range is well suited for heat utilisation from natural geothermal sources. The membranes employed by conventional electrolyzers are of a multi-component formulation that includes binding polymers and hydrophilic elements and are temperature limited, losing structural integrity and saturation capabilities at temperatures past their glass-transition, which is usually ≥ 100°C.

With the absence of a conventional membrane/diaphragm, the core DEFT™ principle provides a potential solution to achieving medium temperature electrolysis. Operating at medium temperature will allow for a significant reduction in the electrical energy required to split water, hence lowering the overall energy consumption of the system.

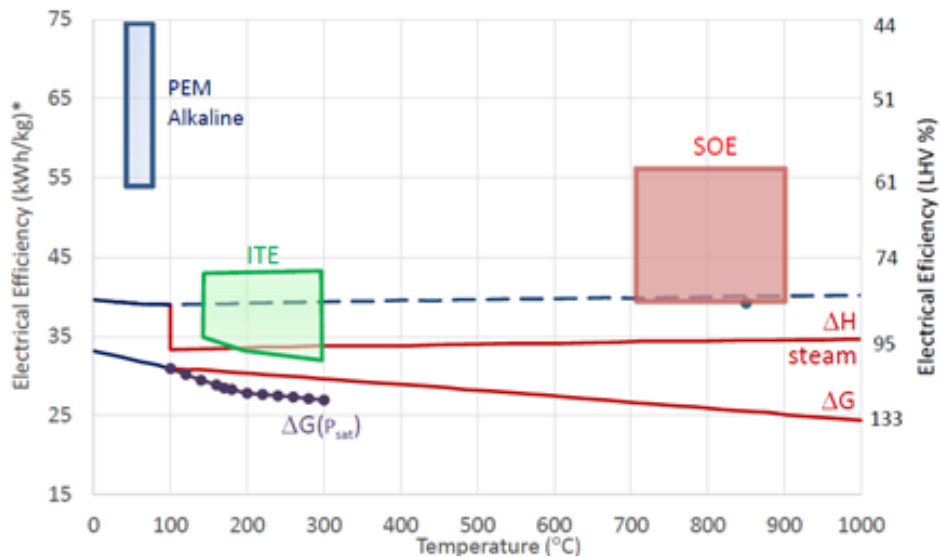


**Figure 7-1: Thermodynamic considerations for the water decomposition reaction**

From Figure 7-1 above, the Gibbs free energy (electricity) contribution becomes substantially lower with increasing temperature as the balance is made up of heat introduced/generated within the system.

This suggests that a medium temperature electrolysis unit can operate at between 20-40% lower electricity consumption compared to mainstream Alkaline and PEM stacks. This can be achieved by operating close to or below (endothermic) the thermo-neutral voltage by supplying waste heat (geothermal / process waste) to the electrolysis system. This would imply an electrical efficiency of close to 100 HHV% or slightly lower if it is still desired that waste heat be utilised within the system to bring it up to operating temperature. The system efficiency, however, will depend on the configuration and associated parasitic loads of the technology. The levelised cost to produce hydrogen can, therefore, be reduced by a further 15-30% as compared to mainstream conventional electrolysis systems.

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## ANNEXURES

### Appendix A – Operating Conditions and Assumptions Associated with the Uses Cases Mentioned in Table 2-10.

#### Hydrogenics: 60 Nm<sup>3</sup>/hr alkaline system.

A study on the progress of Hydrogenics technology and the cost reduction potential for electrolyser technology was conducted by Denis Thomas of Hydrogenics during June 2018. In this study, alkaline and PEM electrolysers were considered in both the kW and MW scale. The data for a small-scale alkaline system was used in the data above. The data reported for the system is not based on project or real-life scenario, but rather on manufacturer information. The capital costs reported are for the hydrogen generating system only, and does not include auxiliary equipment and process, such as storage, cooling, and compression. The given lifespan is the predicted value for this system. As this data was based on manufacturer information, and not on a real project, the electrical costs per kW for this system cannot be determined, as this would vary based on the end-use location of this particular system. As such, the total \$/kg H<sub>2</sub> value, as well as electrical costs for the system cannot be determined. For comparison purposes, a generic electrical cost can be imposed when comparing to DEFT™ 2.5 technology. While the system is considered as 'small-scale', the reported capacity of the system is above the production range of DEFT™ 2.5.

#### Rome Use-Case: 30 Nm<sup>3</sup>/hr alkaline system.

A techno-economic analysis on the in-situ production of hydrogen through water electrolysis and biomass gasification was carried out for a hydrogen fuelling station in Rome. The data for a small-scale alkaline water electrolysis system was analysed to compare to existing electrolysis systems of similar capacity in the Rome HRS site. The specifications of the alkaline electrolyser for this system is identical to that of the Hydrogenics electrolyser, except for the capacity, which is 30 Nm<sup>3</sup>/hr. The CAPEX, consequently, is higher for this system, as it is a lower kW system, in comparison to the Hydrogenics system. The cost per kg hydrogen is at the expected production price of approximately \$7. The average grid electrical cost, which varied according to peak, intermediated and off-peak times in Italy, was recorded as approximately 0.077 \$/kg. This is slightly cheaper than peak rates in South Africa but higher than that of the combined grid and solar energy. As such, the electrical costs contribute the most to the overall production cost (61%) of hydrogen. The lifespan of the plant was reported as 10 years, and CAPEX values did not include auxiliary equipment and process such as compression, cooling, and storage. The

electrolyser was reported to operate for 24 hours per day. The biomass gasification plant was excluded from all data analysis for this investigation.

### **Korean Use – Case: 30 Nm<sup>3</sup>/hr alkaline system**

A theoretical sensitivity analysis for alkaline electrolyser systems was carried out by Korean researchers Lee *et al*, 2017. The technical data used in this study was based on electrolyser systems manufactured by EM Korea. The plant was assumed to operate for years, 365 days per year, and 24-hour days. The original analysis includes cost data for compression, storage, and dispenser capital costs, but this was removed to provide a better comparison to the DEFT™ 2.5 unit. The electrical costs for this system are unusually low, as the calculated electrical rate for this plant is approximately 0,03 \$/kWh; this is still arguably low for a renewable energy source. The CAPEX per kW<sub>installed</sub> of the system is presented as a fairly low figure, but this is due to the high electrical demand of the system. EM Korea's electrolyzers are reported to operate at approximately 78 kWh/kg H<sub>2</sub>. This is reflected, however, in the \$/kg H<sub>2</sub> CAPEX value, as a high 3,7 \$/kg H<sub>2</sub>. The OPEX values are high due to maintenance costs that occur each year. Furthermore, the CAPEX values of this system are inclusive of compression equipment, as well as including the associated electrical consumption costs. This is possibly why the CAPEX costs are slightly greater than the expected value for the system.

### **Norwegian Use-case: 30 Nm<sup>3</sup>/hr PEM system.**

A study on the use of a small-scale PEM electrolysis system in a hydroelectric system was conducted by Ulleburg and Hancke, 2018, Norway. Two systems were analysed, namely a 30 Nm<sup>3</sup>/hr and a 45 Nm<sup>3</sup>/hr system. For this investigation, data on the 30 Nm<sup>3</sup>/hr system was used. The reported efficiency of the system included compression; however, this electrical consumption was removed from the overall system consumption, to find the electrical consumption of the electrolyser only. The project lifetime was assumed to be 10 years, with a stack lifetime of 90 000 hours. The OPEX costs were assumed to be 4% of the overall CAPEX values. Since the electrolyser is operated in an existing hydroelectric plant, the electrical costs are not included in the overall production cost per kg hydrogen, dropping this value to 4.5 \$/kg H<sub>2</sub>. The exchange rate between the Norwegian NOK and the US dollar is 8,5 NOK to the US\$. The electrolyser system used in this case study presents a lower CAPEX per kW<sub>i</sub> than that of the Rome case study. This is most likely due to the higher electrical consumption of the system, as the total \$/kg CAPEX value is much higher in comparison to the Rome case study. Furthermore, the system costs for the Norwegian system is significantly lower in comparison to the Rome case, which could explain the poor efficiency of the Norwegian system.

**PERIC – 5 Nm<sup>3</sup>/hr alkaline system.**

Technical data for a 2,5 Nm<sup>3</sup>/hr system was made available by PERIC. This is the only data that was obtained for an electrolysis system of comparable capacity to the DEFT™ 2.5 unit. Electrical efficiency and lifespan for the system were not reported, however, A lifespan of 7 years was assumed for the stack, as well as the efficiency of 58 kWh/kg The CAPEX values are high but can be expected for the small capacity of the plant. This value will be the most comparable to that of the DEFT™ 2.5 unit. The plant is assumed to operate for 365 a year, at 24 hours per day.

## Appendix B – Independent Lab Gas Purity Tests for the BI-MCFP Pilot Plant



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### TEST REPORT

REPORT NO.: AS-18-280  
PAGE 1 OF 2

#### SUMMARY

|                                        |                                                                    |                    |                     |
|----------------------------------------|--------------------------------------------------------------------|--------------------|---------------------|
| Customer                               | Hydrox Holdings                                                    |                    |                     |
|                                        | Unit E4, Metropolitan Park, Wakis Street, Strijdom Park, Randburg. |                    |                     |
| Test Required                          | Hydrogen and Oxygen                                                | Study number       | Hydrox 18-280       |
| TEST ITEM                              |                                                                    |                    |                     |
| Description                            | Gas sample                                                         | Condition          | Gas                 |
| Identification                         | H <sub>2</sub> (S1 & S2) O <sub>2</sub> (S1 & S2)                  | Date of Receipt    | 18/10/2018          |
| Number of Samples                      | 4                                                                  | Storage conditions | At room temperature |
| Storage date                           | None – taken from unit and analysed                                | Date of Analysis   | 18 - 19/10/2018     |
| Method/s used                          | Standard methods of Analysis as specified.                         |                    |                     |
| Environmental Conditions with analysis | Temperature: 23 °C Humidity: 38 %RH                                |                    |                     |

#### TEST ITEMS

On 18 October 2018 Airsep Laboratory tested gas samples from Gas Sampling Bags supplied by Hydrox Holdings.

The request was to issue a COA for the gas content in the sample.

Before the start of the analyses, each test item was examined visually to determine if any foreign material was present. Odour, colour and any other physical aspects were noted. A representative sample was taken for analysis.

#### ANALYTICAL METHODS AND TEST GUIDELINES

The methods/instruments used for the analysis are all part of an on-going quality control system and were standardized before the analysis took place.

Analyses was performed with on and Agilent 6890 gas chromatograph with a suitable capillary column. Certified standards were utilized prior and during analysis.

P O Box 7954, Bedfordview 2008. Tel. 011 6152855 Fax 086 7186968 Cell: 0828505891 [airsep@vodamail.co.za](mailto:airsep@vodamail.co.za)

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**CERTIFICATE OF ANALYSIS 18-280**  
**ANALYSIS OF GAS SAMPLES**

| Sample | Test Result (%) |                |                | Uncertainty of result |
|--------|-----------------|----------------|----------------|-----------------------|
|        | H <sub>2</sub>  | O <sub>2</sub> | N <sub>2</sub> |                       |
| "S1"   | 99.81           | 0.05           | 0.14           | ± 0.1 %               |
| "S2"   | 99.70           | 0.10           | 0.20           | ± 0.1 %               |
| "S1"   | < 0.2           | 99.35          | 0.45           | ± 0.1 %               |
| "S2"   | < 0.2           | 99.28          | 0.52           | ± 0.1 %               |

**OBSERVATIONS**

1. The gas was sampled directly from the gas sampling bags supplied before injection directly into the gas chromatograph.
2. Some residual air N<sub>2</sub> may be due to the sampling bags and the injection technique.

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Dr RF van de Water  
 Responsible Laboratory Manager  
 Pr.Sci.Nat. (Practice number 114194)

Date: 19 October 2018

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## Appendix D – XRF Analysis of Electrolytic Sludge

Table E: Powder XRF analysis of electrolytic sludge (mass%)

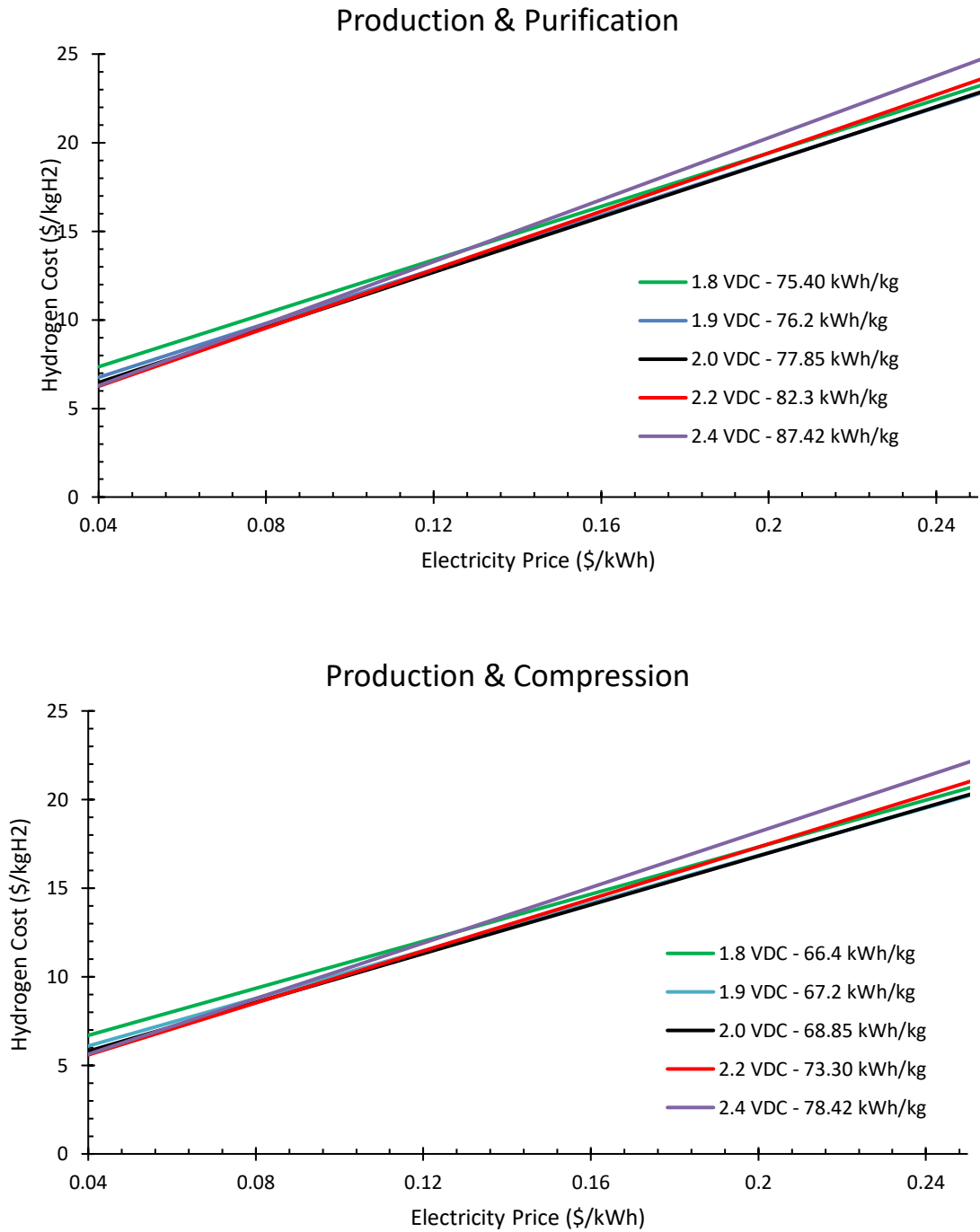
| Element                               | Composition in Mass% |
|---------------------------------------|----------------------|
| Loss on ignition @ 1000°C (Volatiles) | 43.2                 |
| Potassium                             | 25.6                 |
| Nickel                                | 15.8                 |
| Iron                                  | 1.21                 |
| Calcium                               | 0.32                 |
| Aluminium                             | 0.25                 |
| Chromium                              | 0.22                 |
| Magnesium                             | 0.15                 |
| Silicon                               | 0.12                 |
| Zinc                                  | 0.049                |
| Titanium                              | 0.048                |
| Manganese                             | 0.04                 |
| Copper                                | 0.02                 |
| Sulphur                               | 0.016                |

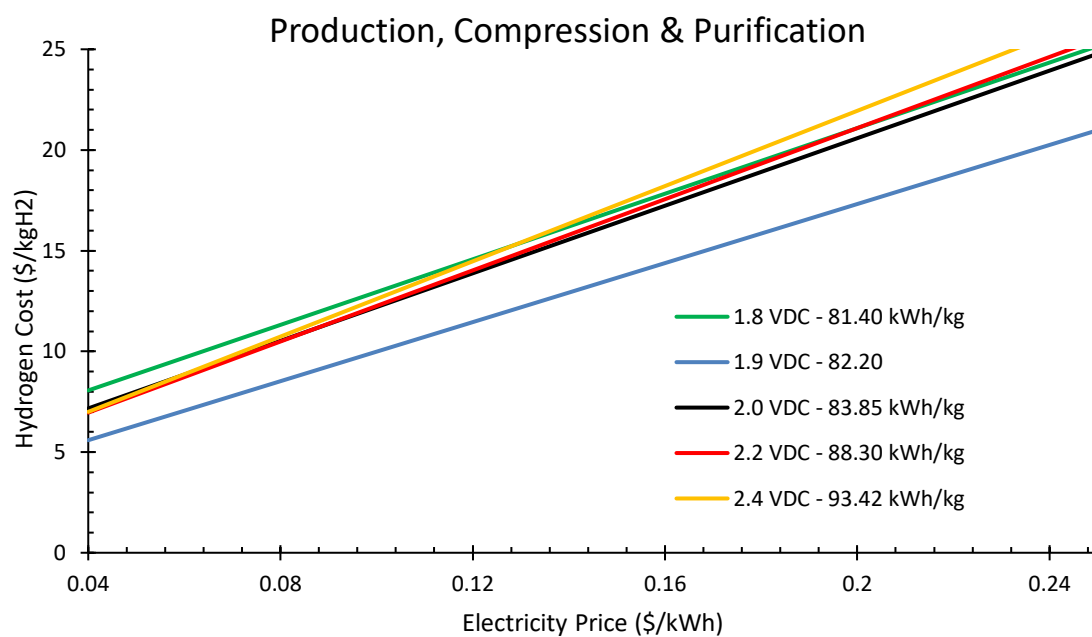
**Appendix E – Bill of Materials for the Construction of the 3 – 5 kg/day H<sub>2</sub> DEFT™  
2.5 Unit.**

| Section                        | Component                         | Cost (R)       |
|--------------------------------|-----------------------------------|----------------|
| <b>Stack</b>                   | Mesh Electrodes                   | <b>33 387</b>  |
|                                | Reactor Gaskets                   | <b>12 884</b>  |
|                                | Reactor Plastic Components        | <b>95 145</b>  |
|                                | Bi-polar plates                   | <b>21 000</b>  |
|                                | Non-Conductive Layer              | <b>1 945</b>   |
|                                |                                   | <b>164 361</b> |
| <b>Electrolyte Circulation</b> | Electrolytic Pump                 | <b>4 899</b>   |
|                                | Heat Exchanger                    | <b>12 969</b>  |
|                                | Dosing Pump                       | <b>8 813</b>   |
|                                |                                   | <b>26 681</b>  |
| <b>Gas Processing</b>          | Gas-Liquid Separators             | <b>104 655</b> |
|                                | Gas Washers                       | <b>53 466</b>  |
|                                | Purge Vessel                      | <b>14 737</b>  |
|                                | Moisture Filters                  | <b>1 148</b>   |
|                                | Reactor/Media Balls               | <b>12 040</b>  |
|                                | Moisture trap                     | <b>5 180</b>   |
|                                |                                   | <b>191 226</b> |
| <b>Piping and Valves</b>       | Piping Components                 | <b>35 824</b>  |
|                                | Piping Labour                     | <b>34 332</b>  |
|                                | Regulators                        | <b>5 163</b>   |
|                                | Magnetic Filters                  | <b>15 120</b>  |
|                                | Flashback Arrestors               | <b>13 070</b>  |
|                                | Solenoid Valves                   | <b>9 100</b>   |
|                                | Ball Valves                       | <b>6 226</b>   |
|                                | Pressure Relief Valves            | <b>2 144</b>   |
|                                | Check Valves                      | <b>3 238</b>   |
|                                | Control Valves                    | <b>6 755</b>   |
|                                |                                   | <b>130 972</b> |
| <b>Plant Electronics</b>       | Metal Work                        | <b>17 826</b>  |
|                                | DC Stack                          | <b>24 150</b>  |
|                                | Electronics                       | <b>14 304</b>  |
|                                | Switchgear                        | <b>15 120</b>  |
|                                | Labour                            | <b>62 100</b>  |
|                                |                                   | <b>133 501</b> |
| <b>Plant Frame</b>             | Framework                         | <b>62 395</b>  |
|                                | Labour                            | <b>38 833</b>  |
|                                |                                   | <b>101 228</b> |
| <b>PLC Control</b>             | PLC Hardware                      | <b>16 300</b>  |
|                                | PLC programming and Commissioning | <b>69 000</b>  |
|                                | PLC Software License & Computer   | <b>24 895</b>  |
|                                | UPS                               | <b>1 834</b>   |
|                                | Variable Speed Drive              | <b>16 760</b>  |
|                                | Rectifier                         | <b>29 400</b>  |
|                                |                                   | <b>158 189</b> |
| <b>Instrumentation</b>         | Pressure Sensors                  | <b>11 369</b>  |
|                                | Level Sensors - Analogue          | <b>16 485</b>  |
|                                | Level Sensors - Digital           | <b>25 123</b>  |

|                         |                                |                  |
|-------------------------|--------------------------------|------------------|
|                         | Temperature Sensor             | <b>3 306</b>     |
|                         | Liquid Flowmeter               | 16 408           |
|                         | De-ionised Conductivity Sensor | 2 304            |
|                         | KOH Conductivity sensor        | 7 853            |
|                         | Capacitance Sensor             | <b>6 725</b>     |
|                         | Fixed Gas Detector             | <b>8 228</b>     |
|                         | Hydrogen Gas Purity Sensor     | <b>27 720</b>    |
|                         | Oxygen Gas Purity Sensor       | <b>27 720</b>    |
|                         |                                | <b>153 241</b>   |
| <b>Water Generation</b> | De-ionised Water Generator     | <b>6 801</b>     |
|                         |                                | <b>6 801</b>     |
| <b>Gas Purification</b> | Gas Purification Plant         | <b>224 000</b>   |
|                         |                                | <b>224 000</b>   |
| <b>Gas Compression</b>  | Compressors                    | <b>127 152</b>   |
|                         | Buffer Tanks                   | <b>20 000</b>    |
|                         | Pressure Sensors               | <b>11 369</b>    |
|                         |                                | <b>158 521</b>   |
| <b>Total</b>            |                                | <b>1 448 722</b> |

**Appendix F – Cost per kg Hydrogen Versus Electricity Price for Different Configurations of the DEFT™ 2.5 Unit.**





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Author: Shihui Zou, Michaela S. Burke, Matthew G. Kast, et al

Publication: Chemistry of Materials

Publisher: American Chemical Society

Date: Dec 1, 2015

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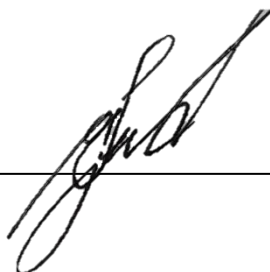
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