## TECHNO-ECONOMICAL ANALYSIS ON THE PRODUCTION OF HYDROGEN

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by

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### ABSTRACT

Hydrogen is an interesting and promising alternative for fuels. Currently, most hydrogen is produced via a process called steam reforming, where a reaction between methane and water occurs, with carbon monoxide and carbon dioxide as waste products and released in the atmosphere. This work presents a study on the sustainable production of hydrogen. A pool of six hydrogen processes were chosen; three based on electrolysis, two based on fermentation and one based on electrolysis combined with a microbial community. On these six methods an early stage analysis was applied, screening for economics, environmental impacts and processrelated costs and impacts.

Two electrolysis methods were selected for a conceptual design; alkaline electrolysis (AE) and polymer electrolyte membrane (PEM) electrolysis, both for an annual production of 1 million kg hydrogen. The fixed capital was established \$86.8M for AE and \$62.3M for PEM. After the design, a techno-economic analysis was performed, providing the total production cost (TPC) and the minimum fuel selling price (MFSP). For the AE, the MFSP resulted in being \$21.46/kg hydrogen and an TPC of \$17.16/kg hydrogen. The biggest contribution to the MFSP was the depreciation, being \$10.19/kg hydrogen. The PEM electrolysis had a MFSP of \$17.56/kg hydrogen and an TPC of \$14.05/kg hydrogen. Also for PEM electrolysis, the biggest contribution to the MFSP was the depreciation, being \$21.40/kg.

A sensitivity analysis was performed and showed the biggest uncertainty in the equipment cost and the interest rate. The MFSP for AE changes  $\pm$  \$3.79/kg hydrogen by a change in equipment cost of 30% and  $\pm$  \$3.27 - \$3.72 by a 5 percentage point change of the interest rate. The MFSP for PEM changes  $\pm$  \$2.73/kg hydrogen by a change in equipment cost of 30% and  $\pm$  \$2.36 - \$2.73 by a 5 percentage point change of the interest rate. Based on the results from the techno-economic analysis and sensitivity analysis, PEM electrolysis was identified as the superior method.

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## 1 INTRODUCTION

The Kyoto Protocol was established as a part of the United Nations Framework Convention on Climate Change (UNFCCC) in 1997. It was formulated to handle the human interference with the climate system and preserve the greenhouse gas concentration in the atmosphere [2]. The protocol came into force from 2005 to 2020 and was succeeded by the Paris Agreement in 2015; which is an international treaty on climate change to limit global temperature rise below 2 °C (preferably below 1.5 °C) above pre-industrial levels. To reach this goal, emissions are ought to be reduced to carbon neutral before 2050 [3]. Moving from fossil fuels to more sustainable energy sources is indispensable [4].

The use of biofuels is an often proposed way for moving to a sustainable alternatives. Although these biofuels are still in technological development and are not always economically viable yet, the feedstock for these biofuels are more locally and widely available. The use of these renewable raw materials do not cause any depletion when used responsibly [5].

A promising biofuel could be using hydrogen as an energy carrier. Hydrogen is able to contain a high amount of energy, with an energy density of 120 MJ/kg. Furthermore, by using hydrogen as a fuel, its only emission product is water vapour [6]. Currently, the production of hydrogen mainly happens by using methane steam reforming; which is a method that utilizes fossil fuels and emits carbon monoxide and carbon dioxide [7]. So besides the clean energy carrier, the production method also needs to be clean and sustainable. This study focuses on the production of hydrogen via electrolysis and fermentation processes.

These production methods based on electrolysis and fermentation are relatively new and not yet applied in big scale production [8]. This work provides information on the techno-economical aspects of these production methods. Literature often provides information on the variable production cost of hydrogen production; this study provides both fixed and variable cost and the eventual minimum fuel selling price (MFSP) to answer the research questions:

- What are the most viable methods for large-scale hydrogen production from a techno-economic perspective?
- What are the major cost contributions for hydrogen productions methods?
- How do variations in key parameters impact the overall production costs?

To answer these questions, a literature research was performed on these production methods. The investigated electrolysis and fermentation processes are introduced and explained in Chapter 2. Chapter 3 explains the methodology and goes into more detail how this assessment was performed. Next, six chosen production methods were assessed in an early state analysis (Chapter 4), showing these results, providing a sensitivity analysis and discussion. Thereafter, two methods were chosen for further research; first providing a conceptual design in Chapter 5 and then

### 2 | INTRODUCTION

analyzed in the techno-economic analysis (Chapter 6). In the techno-economic analysis, results are shown, the outcome of the sensitivity analysis is shown and both are discussed. Finally, after obtaining the results and having them discussed, the research questions can be answered in the conclusion (Chapter 7).

## 2 TECHNOLOGICAL BACKGROUND

Hydrogen is considered to be a clean alternative in comparison to fossil fuels due to the reduction of  $CO_2$  and  $NO_x$  emissions [9]. Hydrogen is able to store energy transported from other energy resources like fossil fuels, water and (wind)electricity; storing energy in the hydrogen molecule as an energy carrier [10].

The earliest references of using hydrogen as energy carrier date from 1838, when Sir William Grove invented the fuel cell [11]. Fuel cells are able to produce water and electricity by providing fuel (hydrogen) and oxygen [12]. However, reversing this process by providing electricity and water in a fuel cell electrolyzer causes an opposite reaction producing oxygen and hydrogen gas; a process called electrolysis. In an electrolysis, water is split into protons and oxygen ions, where the protons move to the cathode and the oxygen ions mitigate to the anode. The negative oxygen ions donate their protons to the positive anode and the protons receive electrons from the negative cathode, forming oxygen and hydrogen gas at either side of the fuel cell [13]. Several methods of the use of electrolysis are explained in this chapter.

A more novel method for the production of hydrogen is the use of microorganisms. Microorganisms are able to use feedstock like sugars and biomass to break it down, producing hydrogen without fossil fuel depletion [14]. Also, the carbon that is emitted at the using these microorganisms is part of the natural carbon cycle [5]. Six methods based on electrolysis, microorganisms or a combination of them are presented in this chapter.

### 2.1 ALKALINE ELECTROLYSIS

Alkaline electrolysis (AE) focuses on the conversion of water to hydrogen; water is being split into hydrogen gas and oxygen by using electric energy (Eq 2.1,2.2,2.3). The set-up of such a electrolysis consists of an anode, a cathode, electric energy and an electrolyte (Figure 2.1) [13; 15]. From a direct current (DC) electrons flow from the negative terminal to the cathode. This negative cathode attracts protons and form hydrogen. To keep the electrical charge in balance, the anode attracts negatively charged anions (hydroxide ions) and form oxygen and water. Because hydrogen and oxygen are formed at opposite sides of the electrolysis, it is rather simple to separate these gasses. Nickel was selected as material for the cathode and anode; this was because of its high activity, high availability and low cost. An alkaline solution of sodium or potassium hydroxide (30%) is commercially often used as electrolyte [13]. AE typically operates at temperatures ranging from 60°C - 90 °C and at pressures up to 30 bar. Typical current densities range from 0.2-0.4 A/cm<sup>2</sup> and an operating cell voltage of 1.8-2.0 V [13; 16]. AE is considered to be a mature technology and suitable for scalability [17; 18].

$$Cathode: 2H^+ + 2e^- \to H_2 \tag{2.1}$$

Anode: 
$$2OH^- \to 0.5O_2 + H_2O + 2e^-$$
 (2.2)

$$Overall reaction: H_2O \to H_2 + 0.5O_2 \tag{2.3}$$



Figure 2.1: A schematic illustration of a basic water electrolysis system.

### 2.2 PROTON EXCHANGE MEMBRANE ELECTROLYSIS

Another method to use electrolysis to produce hydrogen is using a proton exchange membrane (PEM) (Figure 2.2). PEM is an established hydrogen production method with a growing technological maturity [17; 18]. In the PEM, the membrane is used as electrolyte. At the anode of the PEM, a water molecule is split in oxygen and protons. This process is similar to AE, but in this case a polymer made of perfluorosulonic acid (Nafion<sup>*TM*</sup>) [19] can be used as a membrane that let only protons pass from the positive anode to the negative cathode. The polymer provides a high proton conductivity and a low gas crossover. Due to the inability of gas to cross the membrane, only protons cross the membrane and hydrogen is yielded with high purity [20]. The anode and cathode are made from stainless steel, with the anode having a thin layer of iridium oxide as catalyst and the cathode using a thin platinum layer as catalyst. The operating temperature varies from 50 °C - 80 °C, with varying pressure from 1-30 bar. PEM electrolyzers operate at current densities ranging from 1-2 A/cm<sup>2</sup> and using a cell voltage of 1.8-2.2 V [20; 21].



Figure 2.2: Schematic representation of PEM electrolysis

### 2.3 SOLID OXIDE ELECTROLYZER CELL

The solid oxide electrolyzer cell (SOEC) is a operating system that produces hydrogen at high temperatures; namely between 500 and 1.000 °C. At these temperatures, steam is fed instead of water together with  $CO_2$ . The operating system of a SOEC consists of a dense ionic conducting electrolyte and two porous electrodes (Figure 2.3). After steam and a electrical potential is applied to the system, water molecules diffuse through the porous cathode to the electrolyte. At the interface of the electrolyte the water molecule receives two electrons and dissociates into hydrogen gas and oxygen ions. The oxygen ions are transported through the electrolyte and at the porous anode, the oxygen ion donates its electrons and oxygen gas diffuses through the porous anode (Eq 2.4,2.5,2.6). Although SOEC is a promising technology, it is considered to be a less evolved production method and requires more research before becoming commercially available for big scale production [17; 22].



Figure 2.3: Schematics of SOEC hydrogen production.

The net reactions for the cathode are:

$$H_2O(g) + 2e^- \rightarrow H_2(g) + O^{-2}$$
 (2.4)

For the anode:

$$O^{-2} \to 0.5O_2 + 2e^-$$
 (2.5)

The overall reaction:

$$H_2O \to H_2 + 0.5O_2$$
 (2.6)

### 2.4 MICROBIAL ELECTROLYSIS CELL (MEC)

The Microbial Electrolysis Cell (MEC) is a method that uses both renewable energy and microorganisms. In this cell (again with an electrical power source, anode and cathode), microorganisms are anchored to the anode (Figure 2.4). The material of the anode can be carbon (cloth or paper) or graphite [23] (granules or brushes). The microorganisms at the anode, typically consisting of acetate oxidizing bacteria as *Geobacter* species, consume the substrate (acetate) as carbon and energy source [24]. The substrate is oxidized and it releases its electrons that flow through the circuit

to the cathode, generating an electric current. At the cathode, the protons are combined with the electrons from the anode side and form hydrogen gas [25].

Acetate is a viable feedstock for the Microbial Electrolysis Cell [24]. Besides it ability to support the microbial growth, it is also a feedstock that is widely available and biodegradable. Also, since acetate can be derived from waste streams or from  $CO_2$  [26; 27], it makes it a sustainable and cheap feedstock. The MEC operates at the optimal temperature for the microorganisms, which is often slightly more than room temperature and operates at atmospheric pressure [23].



Figure 2.4: Schematics of MEC hydrogen production.

### 2.5 DARK FERMENTATION

The first of the two completely biobased methods discussed in this thesis is dark fermentation (DF). In the last decade, secondary feedstocks have gained more interest as a feedstock for biobased processes. The DF method within this thesis considers corn stover as a feedstock; after a pretreatment with calcium hydroxide (Ca(OH)<sub>2</sub>) glucose and xylose are produced. Subsequently the glucose and xylose are used as feedstock for a dark fermentation [28; 29].

Microorganisms are implemented to help with the conversion of these complex waste substrates. Microorganisms are capable of using energy-rich hydrogen molecules and use the electrons from the oxidation of hydrogen to produce energy [30]. The microorganisms during the DF are kept under anaerobic conditions and in absence of light (hence the name of this method). The temperature of this process is dependent on the microorganism, but is often carried out within the range of 25-80 °C [30]. The products of the DF, besides hydrogen, are  $CO_2$  and volatile fatty acids (VFA) like acetate or butyrate [30; 31; 32].

Lignocellulosic biomass is able to provide glucose and xylose after hydrolyzation. Corn stover is an agricultural wastes that might be able to provide a considerable amount of sugars, to be used in hydrogen producing systems. The glucan and xylan of the lignocellulosic biomass is treated and hydrolized; this results in glucose and xylose [28; 33].

The thermophillic bacterium *T. thermosaccharolyticum* W16 has been selected as microorganism for the production of hydrogen in the dark fermentation, with optimal pH and temperature 6.5 and 60°C respectively [29]. The feedstock for this organism can be a mixture of glucose and xylose. This results in the production of not only  $CO_2$  and hydrogen, but also acetate and butyrate (Equation 2.7, Equation 2.8) [29; 34].

Eventhough the theoretical maximum hydrogen yield is 4 mol  $H_2$ /mol glucose, the experimental yields lay lower due to microbial growth.

Dark Fermentation:

$$C_6H_{12}O_6 + 6H_2O \rightarrow 2CO_2 + 4H_2 + 2CH_3COOH$$
 (2.7)

$$C_6H_{12}O_6 + 6H_2O \rightarrow 2CO_2 + CH_3CH_2CH_2COOH + 2H_2$$
 (2.8)

### 2.6 PHOTO FERMENTATION

In the case of photo fermentation (PF), which is performed under anaerobic conditions and solar light, carbohydrates or organic acids are converted into hydrogen and  $CO_2$ . The phototrophic bacteria (like *Rhodobacter sphaeroides*) possess the ability to absorb light energy (photons) and store it as chemical energy [35]. Excitation energy is used to transmit one electron from a chemical compound (donor) to another compound (acceptor). So the electrons from the donor are pumped through some of the electron carriers, over the membrane; ATP is synthesized due to a proton gradient. A nitrogenase utilizes the energy from the ATP to reduce the protons into hydrogen gas. Because of the oxygen sensitivity of nitrogenase in this process, it is important the reaction takes place under anaerobic conditions [36; 37].

The PF typically uses carbohydrates or organic acids as feedstock for this fermentation. Acetate is an applicable substrate for the PF due to its wide availability and low production cost. The phototrophic bacterium *Rhodobacter sphaeroides* possesses the enzymes and metabolic pathways to utilize acetate as substrate and produce hydrogen gas at atmospheric pressure and temperature of 25-30 °C [38; 39].

## 3 | METHODOLOGY

After a screening process focused on efficiency, feedstock source, by-products and costs, six methods were selected, which were introduced in the literature research of Chapter 2. The purpose of this thesis is to research the most techno-economically viable production methods for big scale hydrogen production. The technological aspects and the economical viability of these methods are researched in this thesis.

To get a better perspective on the six production methods, a multi-criteria evaluation combined with a sensitivity analysis were performed. In the early stage analysis six methods are assessed on both economical and environmental pillars. After this early stage analysis, two methods were selected for conceptual process design and further assessment in the techno-economical analysis, where the total cost and the manufacturing fuel selling price were determined.

### 3.1 EARLY STAGE ANALYSIS

Since the last couple of decades, sustainability has become a more important value to (chemical) businesses. Prior to this, economic performance was considered the most important value in decision making. As new (bio-)chemical production methods are being developed, it is important that these new methods are analyzed by not only a techno-economic pillar, but also an environmental and social pillar. The early stage analysis is used to provide this information [40; 41]. The work of Patel et al. [40] was used as an important basic principle in this thesis. The economic and environmental pillars in his paper were used and adapted to an assessment for analyzing various methods for the production of hydrogen.

The assessment methodology is divided into several parameters that are explained in the following paragraphs.

#### 3.1.1 Methodology description

The methodology as constructed by Patel et al. [40] contains five parameters that contribute to a final score: *Economic constraint* (EC), *environmental impact of raw materials* (EI), *process costs and environmental impact* (PCEI), *Environmental, Health & Safety* (EHS Index) and *Entrepreneurial risk aspects* (RA). However, recent studies have disclosed that the EHS index and the RA are to be excluded due to the high uncertainties and relatively high effort that has to be put in for research objectives [42; 43]. Therefore, this research will rely on the three pillars: the EC, EI and PCEI parameters.

For commercial implementation of a certain hydrogen production method, economical feasibility is of high priority; since a process will not be implemented if there is no profit to be gained. Therefore, a market price will be established that includes the cost of the raw material and production costs. The *economic constraint*  (Equation 3.1) describes the ratio of the raw material costs regarding to the value of the products and possible co-products that are to be sold.

Economic Constraint(EC) = 
$$\frac{\sum_{i=1}^{r} m_i \cdot C_i}{\sum_{j=1}^{p} m_j \cdot C_j}$$
(3.1)

In Equation 3.1 the mass flow is multiplied with the market price of each raw material (r) or (co-)product (p). The variables  $m_i$  and  $C_i$  describe respectively the mass flow and the commercial prices of the *i*<sup>th</sup> raw material;  $m_j$  and  $C_j$  represent respectively the mass flows and prices of the *j*<sup>th</sup> product. A low ratio (< 1) means that the sum of the economic value of the raw materials is lower than the value of the profit and thus leaves more (financial) room for investing in capital and process costs.

Beside the pillar of the economic constraint, this thesis also assesses the environmental pillar with the focus on the raw material: *Environmental impact of raw materials* (Table 4.3). The EI is composed of two elements: the Cumulative Energy Demand (CED) and the Global Warming Potential (GWP). The CED portrays the total energy requirements used for the production of the raw materials. These energy requirements are based on the higher heating values of the energy sources (e.g. natural gas, wind). The scope within this assessment is a cradle-to-gate approach; also a possible location was considered to be in Europe.

Subsequently the GWP was also included in this assessment. The GWP provides an indication for the use of non-renewable resources in  $CO_2$  equivalents. The GWP includes estimations based on a 100-year time horizon using the IPCC 2014 GWP 100 method [44].

The CED and GWP results have been obtained via the ecoinvent 3.5 database in SimaPro 9.4 [45]. Both of these scores have been normalised and were given an equal weighing factor ( $w_i$ ) of 0.5. After multiplying the  $w_i$  with the CED and the GWP, both normalized values are summed up, resulting in the EI (Equation 3.2).

Environmental Impact of Raw Material (EI) =  $w_{CED} \cdot CED + w_{GWP} \cdot GWP$  (3.2)

The third pillar of the early stage analysis is the *Process Costs and Environmental Impact* (PCEI). This parameter helps to give an indication on the costs and (environmental) impacts associated with the reaction and products. The energy and mass loss in the reaction and separation stages of the process are used as indicator for the expected costs and environmental impacts. For the PCEI seven indicators are scored based on the data from the reaction. Individual index values are pointed out varying from o to 1 as shown in Table 3.1. The mass loss index (MLI) (Equation 3.3) and the number of co-products were used to determine the downstream complexity. The other five categories notify the complexity of the operating conditions[40; 46].

$$MLI = \frac{\sum_{i=1}^{n} M_i}{\sum_{j=1}^{n} M_j}$$
(3.3)

In Equation 3.3, the  $M_i$  portrays the masses of the starting materials and  $M_j$  represents the masses of the product. The MLI provides information on the mass loss, which is considered to be loss of waste and not converted reactants in the reaction. Furthermore, each of these seven parameter are given the same weight factor. Since the sum of all the weight factors is equal to 1, no normalization step is necessary.

	8	
Indicator	Equation	Internal weight factor
Processing cost and environmental impacts	$PCEI = \sum_{i=1}^{PCEIc} IWF_i \cdot PCEI_i$	
-	$PCEI_1 = 0.0$ , if water is NOT present	
	0.5, if water IS present	0.143
	1.0, if water must be distilled	
	$PCEI_2 = 1 - (1/2)(log_5(100 \cdot c_n))$	
	$PCEI_3 = 1 - (1/2)(log_2(\Delta T_{bp}/5))$	0.143
	$PCEI_4 = (1/2)(log_{10}MLI + 1)$	0.143
	$PCEI_5 = ( \Delta H^0_{R_{YN}}  - 100)/200$ , if $: \Delta H^0_{R_{YN}} \ge 0$	0.143
	or if: $\Delta H_{Rxn}^0 < 0$ and $T_R < 200^\circ C$	0.143
	+ $(100 -  \Delta H^0_{R_{YN}} )/200.$	
	when: $\Delta H_{R_{TR}}^0 < 0$ and $T_R > 200^\circ C$	
	$PCEI_6 = -0.015 \cdot N_{CP}^2 + 0.28 \cdot N_{CP} - 0.25$	0.143
	$PCEI_7 = 0$ , if feedstock pretreatment is NOT required	0.143
	1, if feedstock pretreatment IS required	

Table 3.1: C	ategories	of PCEI
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Note: C: commerical price or cost (k/kg), c: concentration (mol/mol), IWF: internal weight factor, MLI: mass loss index,  $N_{CP}$ : number of co-products,  $\Delta H^0_{Rxn}$ : standard enthalpy of reaction (kj/mol),  $\Delta T_{bp}$ : smallest absolute difference between the boiling point of the product and another substance that has to be separated form this product (°C), Sub-indexes: i, j, n: counter for species i, j and main product

#### 3.1.2 Normalization and weighting

The calculated parameters for the EC, EI and PCEI are not directly on a comparable level and thus cannot be added together yet. First the scores were normalised by the highest (and thus the most unfavourable) value. The highest value divided by that same highest value will result in a score of 1; the other scores will be between o and 1. Equation 3.4 explains this with the EC as example [40; 46]. Subsequently, each of these normalised values were multiplied by the corresponding weight factor. These weight factors are 0.4, 0.3 and 0.3, respective order for the EC, EI and PCEI [40; 46; 47].

$$EC_n = \frac{EC}{\max(EC)}$$
(3.4)

#### 3.1.3 Sensitivity analysis

After the early stage analysis, a sensitivity analysis was performed. This is necessary since every data input is associated with an uncertainty. A variation of data inputs that could change over time (e.g. yields can vary in practice and market prices are dependent on numerous variables). Besides the uncertainty in the data, the values given to the weight factors are also just numbers based on peoples opinions and expertise's and is thus highly sensible. Therefore it is essential to analyze the sensitivity and uncertainties in the outcomes of the early stage analysis [40; 46].

The assessment of the sensitivity analysis was executed by using Microsoft Excel. In this Excel file the aggregated scores of the early stage analysis were calculated and analyzed on the uncertainty in market prices, cumulative energy demand values and global warming potential values. The market price, CED and GWP values may differ for each substrate, so each of these values were up- and down regulated by 50%, aggregated and then plotted as error bars in the plots. Subsequently, the impact of the weight factors were assessed. Also for this assessment an Excel file was utilized. For aggregated scores it was checked what would happen if the combination of weight factors changed, this was done in increments of 10%. The total value for the three weight factors is 1.0, so for the visualization of the effect of the weight factors a ternary plot was created.

### 3.2 TECHNO-ECONOMIC ANALYSIS

After completing the conceptual design, the designed methods were analysed on their economic performances by using a techno-economic analysis. The concept design provided the material balances and energy balances. Based on these balances and the required annual production, equipment sizing was chosen.

In such economic analysis, the capital expenditures (CAPEX) to build the hydrogen production plant and the annual operational expenditures (OPEX) are used to determine the expected lifetime of the plant. The capital costs are mainly based on the required equipment. The equipment cost were retrieved by a literature study; the findings were based on Coulson & Richardson's Chemical Engineering Vol. 6, matche.com [1; 48]. The cost of the electrolyzer was based on the cost (\$) per MW, based on Saba et al. [49]. The dimensions in the process design, equipment sizing calculations were executed and therefore price corrections were performed using the 6/10 rule (Equation 3.5) [50]; where  $C_1$  an  $V_1$  are the known cost (\$) and volume (m<sup>3</sup>) of the equipment,  $C_2$  and  $V_2$  are the cost and volume of the sized equipment.

$$C_2 = C_1 (\frac{V_1}{V_2})^{0.6} \tag{3.5}$$

Once the estimated equipment costs are known, an estimation of the CAPEX can be made. This will be executed by multiplying the estimated equipment cost by the Lang factor [51], as given in Equation 3.6.

Total CAPEX = 
$$\sum$$
 (Total equipment cost) · Lang Factor (3.6)

The value for the Lang factor is dependent on the type of plant. Lang developed factors for plants based on fluid processing, solid processing, and both combined. The values of these factors are 5.93, 4.67 and 5.03 [52], in respective order. Since the electrolysis methods, MEC and dark- and photo fermentation mainly processes fluids (water/acetic acid), these methods use the fluid Lang factor.

After calculating the estimated capital expenses, the operational expenses (OPEX) were established. The OPEX can be divided into variable and fixed expenses. Fixed OPEX are expenses that stay the same, regardless of how much the plant is producing. Examples of fixed OPEX are maintenance cost and labour cost. The variable OPEX are costs that are directly related to the production volume; by increasing production, the variable OPEX will also increase. Examples of variable OPEX are the cost for the raw material and electricity cost. The estimated operational expenses are based on the methodology described in Coulson & Richardson's Chemical Engineering Vol. 6 [1]; Table 3.2 gives a quick overview of the assumptions for estimating the operational expenses. The raw material and utility expenses were based from several sources.

To establish whether the hydrogen production methods make profit, a Net Present Value (NPV) is used to test the economic performance. The NPV is a financial metric that provides the value of the total generated profit [53]; so the profit over the

### Table 3.2: Summary of the assumptions made for estimating operational expenditures(OPEX), based on typical values reported in Coulson & Richardson's [1].

Variable OPEX	Assumption
1. Raw materials	from flow-sheet
2. Miscellaneous materials	10 % of item (5)
3. Utilities	from flow-sheet
4. Shipping and Packaging	negligible

### Fixed OPEX

5. Maintenance	10 % of fixed capital
6. Operating labour	1.9 % of fixed capital
7. Laboratory costs	20 % of item (6)
8. Supervision	20 % of item (6)
9. Plant overheads	50 % of item (6)
10. Capital charges	15 % of fixed capital
11. Insurance	1 % of fixed capital
12. Local taxes	2 % of fixed capital
13. Royalties	1 % of fixed capital

Additional OPEX

14.	Sales	expens	se
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- 15. General overheads
- 16. Research and development

20 % of (variable OPEX

+ fixed OPEX

 Parameters	Value
Project lifetime	20 years
Process operating time	8000 h a <sup>-1</sup>
Start-up costs	20 % of OPEX
Tax on revenues	25 %
 Interest rate	10 %

 Table 3.3: Parameters for the economic model.

total lifetime of the plant. Nevertheless, the NPV only provides information about the profit with a fixed price; while prices during the course of the plants lifetime will most likely shift. An approach to determine the economical viability is establishing the minimum fuel selling price (MFSP) [54]. The MFSP is the break-even selling price where all expenses are paid, but the NPV is zero.

To be able to calculate the minimum fuel selling price (MFSP), certain parameters were required. These parameters are displayed in Table 3.3. With these parameters, the annual depreciation can be calculated by using Equation 3.7; where D portrays the annual depreciation,  $C_{SU}$  is the start up costs, *i* is the interest rate and LT stands from the project lifetime.

$$D = (C_f + C_{SU}) \cdot \left(\frac{i \cdot (1+i)^{LT}}{(1+i)^{LT} - 1}\right)$$
(3.7)

With the calculated annual depreciation, the total production costs per unit (TPC) can be calculated with Equation 3.8.  $R_a$  stands for additional revenues from selling the co-products (like oxygen from electrolysis), *mp* denotes the annual production mass.

$$TPC = \frac{D + OPEX - R_a}{mp}$$
(3.8)

After calculating the TPC, all the parameters are known to estimate the MFSP. Besides the TPC, the local taxes on revenue (T, with T < 1) is taken into Equation 3.9. With the calculated MFSP, prices in literature can be compared for economical feasability.

$$MFSP = TPC \cdot (1+T) \tag{3.9}$$

This chapter describes and discusses the results of the early stage analysis. This section embodies three parameters: the Economic Constraint (EC), Process Costs and Environmental Impact (PCEI) and the Environmental Impact of Raw Material (EI).

### 4.1 RESULTS

As described in Section 3.1.1, an EC value < 1 is potentially profitable and thus more likely to be a promising option. The EC values are calculated as \$ raw materials / \$ products. For the calculation of the EC, the price of hydrogen was set at \$6,-/kg [55]. The mass balance for the production methods are shown in Table 4.1. Alkaline electrolysis (AE), solid oxide electrolyzer cell (SOEC) and proton exchange membrane (PEM) electrolysis all produce oxygen gas as by-product, with pure oxygen having a selling price of \$4.40/kg [56]. Also, the dark fermentation produces acetate (\$1.37/kg) [57] and butyrate (\$1.80/kg) [58] as by-products. The raw material for the AE, SOEC and PEM is distilled water (\$1.02/kg) [59]; distilled water is required to prevent contamination of the electrolyte and potential efficiency [60]. The corn stover used for the dark fermentation costs \$0.15/kg [61].

Process	Mass Balance	Enthalpy Balance
AE, SOEC and PEM	$2H_2O(l) \rightarrow 2H_2(g) + O_2(g)$	$\Delta H = 286  \text{kJ/mol}$
Microbial Electrolysis Cell	$C_6H_{12}O_6 + H_2O \rightarrow CO_2 + H_2$	$\Delta H = 290  \text{kJ/mol}$
Dark Fermentation	$C_6H_{12}O_6 + H_2O \rightarrow 2CO_2 + 2CH_3COOH + 4H_2$	$\Delta H = 215  \text{kJ/mol}$
Photo Fermentation	$CH_{3}COOH + H_{2}O + Light \rightarrow 2CO_{2} + 4H_{2}$	$\Delta H = 272  \text{kJ/mol}$

Table 4.1: Mass and enthalpy balances for various hydrogen production methods

The results for the EC displayed in Table 4.2 show that all six methods have a value lower than 1. This indicates that all six methods have relative low costs for the raw materials inflow, with AE showing the lowest expenses.

The environmental impact of the raw materials comprises of the Cumulative Energy Demand (CED) and the Global Warming Potential (GWP). The results are shown in Table 4.3. Both CED and GWP parameters show the lowest impacts for the AE, SOEC and PEM. The MEC, DF and PF also show low impacts, however, these are relatively higher in comparison with the first three methods.

Table 4.2: Economic constraints	
Method	EC
AE	6.18E-04
SOEC	5.62E-02
PEM	5.33E-03
MEC	4.18E-00
DF	7.11E-01
PF	2.00E-00

Table 4.3: Environmental impact			
Method	CED (MJ/MJ)	GWP (Kg CO <sub>2</sub> eq./MJ)	
AE	7.81E-6	3.59E-5	
SOEC	7.03E-6	3.23E-5	
PEM	2.45E-5	1.13E-4	
MEC	4.04E-2	2.45E-1	
DF	8.62E-2	1.50	
PF	5.86E-2	1.02	

The process related cost and environmental impact (PCEI) is shown in Table 4.4. All six methods show a relative small impact, since a score lower than 1.0 would be favourable. The electrolysis methods AE, SOEC and PEM show the most impactful results.

Method	PCEI
AE	0.21
SOEC	0.13
PEM	0.13
MEC	0.37
DF	0.29
PF	0.28

Table 4.4: Process related cost and environmental impact

The aggregated process scores after normalisation and weighting are shown in Figure 4.1. These results show that AE, SOEC and PEM present the lowest process scores and therefore the most favourable.

### 4.2 SENSITIVITY ANALYSIS

A sensitivity analysis was performed on the results of the early stage analysis. As mentioned in Section 3.1.3, an up- and down regulation of 30% was performed on EC, CED and GHG. The data with the highest sensitivity were shown in the market prices and the assigned weight factors. A  $\pm$  30% price sensitivity on the feedstock



Figure 4.1: Aggregated scores after normalisation and weighting

prices was performed; this uncertainty is shown by the error bars in Figure 4.2. When looking at the error bars for the market price sensitivity analysis, it becomes evident that there is a high uncertainty in MEC, DF and PF. On the other hand, the uncertainty for the market prices is quite low for AE, SOEC and PEM electrolysis.

Beside the sensitivity on the feedstock market price, a sensitivity analysis was performed on the CED and GWP values. These scores were up- and down regulated by 50%, but with smaller deviation ranges. These results are shown in Section A.1 in the appendix.



Figure 4.2: Price sensitivity on feedstock market prices

Additionally, the sensitivity of the weight factors used in the early stage analysis were examined. The weight factors used in this thesis are 0.15 for the CED, 0.15 for the GWP (which result in a total of 0.3 for EI), 0.4 for the EC and 0.3 for the PCEI [42; 46]. The sensitivity analysis provides more information about the combination of weight factors (which sums 1.0), varied over 66 different sets of weight factors, with an increment of 0.1. The results of this analysis are shown in the ternary plots (Figure 4.3). Figure 4.3a shows the results of the best production method with different weight factors. Figure 4.3b shows the second best results and Figure 4.3c the third choice for the hydrogen production methods at different weight factors. The stars in these figures represent the combination of weight factors used in the early stage analysis; EC=0.4, EI=0.3 and PCEI=0.3.



Figure 4.3: Sensitivity on the weight factors, showing the first, second and third choice.

The first choice ternary plot shown in Figure 4.3a displays an almost completely green plot, meaning that for the weight factor EC, EI and PCEI combinations, the PEM electrolysis denotes to be the most attractive method, both from and economic and environmental perspective.

The second choice is more divided in comparison to the first choice. The left side of the plot, which corresponds with an EC lower than 50%, shows a lower score for SOEC. However, when an EC value higher than 50% is chosen, the AE is advised as the second choice. This indicates that the decision making process driven by environmental considerations leads to the SOEC technology. The third choice is then again divided between SOEC and AE, only to show a preference for AE with a low EC (lower than 50%) and an preference for SOEC with an EC higher than 50%. Although SOEC and PEM showed similar results in the early stage analysis, it is shown in these plots that the weighting factors favour one method over the other.

### 4.3 DISCUSSION

During this research, six methods were assessed to identify what technology would have the best potential, from a technical, economic, and environmental perspective, as a possible method for the production of hydrogen. For this assessment, the economic constraints, environmental impact and process related environmental impacts were used as parameter. The results in Table 4.2 show relatively low scores for the first three electrolysis methods (AE, SOEC and PEM) in comparison with the latter three microbial methods (MEC, DF and PF). An important factor for the low scores of the electrolysis methods is the fact that the only feedstock for the electrolysis methods is water; the only produced by-products are oxygen and CO<sub>2</sub>.

Whereas the microbial processes have more complex feedstocks which leads to a higher economic constraint for these microbial based methods.

The parameters for the environmental impact (CED and GWP) Table 4.3 are also based on the amount of feedstock required for 120 MJ (1 kg  $H_2$ ). It is in this situation also visible that the microbial methods show a higher score for the CED and GWP in comparison with the feedstock of the electrolysis (which is water, albeit different volumes). Therefore it is a reasonable result that the AE, SOEC and PEM show lower scores in comparison than the MEC, DF and PF.

All six methods show relatively low scores for the PCEI. With the lowest scores for SOEC and PEM (PCEI = 0.13) and the highest score for MEC (PCEI = 0.37). The most impactful category within the PCEI is the mass loss index (MLI), which can be explained by the fact that the microorganisms use a part of feedstock for maintenance.

After performing an early stage analysis, it becomes clear that the electrolysis methods had the lowest scores and the microbial methods had scores that were way higher. Adjacent to the early stage analysis, a sensitivity analysis was performed. One result that stands out was that the sensitivity for the photofermentation, which is slightly higher than 1.0. The chosen method for the photofermentation demands a high amount of feedstock per kg hydrogen; therefore a high price sensitivity would be a logical result. Moreover, even if the index score would surpass 1.0, it would not mean that the method is insufficient. It merely means that the current advantages are not substantial, but that technological improvements or a lower price would lead to a better performance. The price sensitivity of the AE, SOEC and PEM show a low uncertainty, this is the result of the low cost of the feedstock. The sensitivity of dark fermentation shows also a low uncertainty, this is caused by the low price and relative quantity of the feedstock. The MEC shows a higher uncertainty; the higher price and quantity results in a higher price sensitivity.

During the sensitivity analysis, not only the pillars of the early stage analysis were analyzed, but also the weight factors; this was done and shown by the ternary plots in Figure 4.3. The combination of weight factors used in the early stage analysis is shown with the stars. The most favourable method according to the uncertainty analysis shown in the ternary plot is the PEM electrolysis. With sequential variations of 10%, PEM is still showing in the biggest (middle) part of the plot the lowest scores. Only when EC is not taking into consideration, SOEC is favoured. Additionally, when PCEI is not taken into consideration, AE is the better choice. Overall, when looking at these results, the most favourable choice for further research according to this plot would be PEM electrolysis.

For further analysis in this thesis, AE and PEM electrolysis have been selected. Despite promising results, it was decided not to continue with the concept design and techno-economic analysis for SOEC. SOECs are in earlier stages of technological development, where AE and PEM are more mature methods and seems to be easier scalable in the near future [17]. So for further analysis on process design and techno-economic evaluation, the AE and PEM electrolysis were selected.

## 5 CONCEPTUAL PROCESS DESIGN

After the screening in Chapter 4, two methods were chosen for further research. Before covering the techno-economic assessment, a concept design was made for two electrolysis methods: the alkaline electrolysis (AE) and polymer electrolyte membrane (PEM) electrolysis. This chapter provides a look at a simplified process flow model; where the flowsheet, separation and recycling steps within the system are shown. Both electrolysis methods use a stack of cells. A single cell is only able to produce a limited amount of hydrogen, while a stack of multiple cells increase the total capacity of the electrolyzer [62; 63].

Currently the largest operating alkaline electrolyzer has a total capacity of 20 MW [64] and the biggest PEM electrolyzer operates with a total capacity of 10 MW [65]. The electrolyzers in this study are set at a capacity of 6.67 MW to produce 1 million kilograms of hydrogen per year. Setting the target at 1 million kg per year places the capacity of large-scale industrial projects. To accomplish the goal, a continuous production is required to maintain an operational system with constant quality.

The upstream of the electrolysis methods require a supply of deionized water. The water is free from dissolved minerals, which protects the system from reducing efficiency, equipment failure and electrode protection [15; 66]. Therefore an ion exchange water filter is included in the production system. At the downstream, the produced hydrogen and oxygen leave the condenser at room temperature and atmospheric pressure; to store these products, lower temperature and higher pressure would be required, but this is not included within the scope of this thesis.

### 5.1 ALKALINE STACK

A conceptual design for alkaline electrolysis was made and is shown in Figure 5.1. Water is first deionized by the ion exchange water filter and enters the electrolysis cell stack. The water molecules are decomposed into hydrogen and oxygen through electrochemical reactions. The stack consists of 700 cells with an active surface area of 2.1 m<sup>2</sup> per cell and takes place at 7 bar and at 75°C [67; 68]. An input stream of KOH enters the cell stack, to keep the KOH concentration at 35%. The power (W) input to the stack is 50 kWh for the production of 1 kg hydrogen [69]. The electrolysis produces heat (Q) which is removed by the cooling system. The anode and cathode are both made of perforated carbon steel with a layer of nickel [67]. Oxygen is being formed at the anode and hydrogen at the cathode, resulting in two streams. These streams also contain the electrolyte, which is removed from the gas stream by using a condenser, remaining a 99.9% hydrogen gas and 99.9% oxygen stream [68; 69].

### 5.2 PEM STACK

The method using a proton exchange membrane electrolysis Figure 5.2 also begins with using an ion exchange water filter to deionize the incoming water. The deionized water enters the PEM stack, where the electrolysis takes place at 55°C and 20 bar [67]. The energy input of the system is electrical power, which is 50 kWh/kg



**Figure 5.1:** Conceptual design for Alkaline electrolysis. W = electric power input, Q = thermal power, or heat transfer

hydrogen [70]. This 6.67 MW design has a stack size of 1,000 cells, with an active surface area of 0.1 m<sup>2</sup>. The material for the anode is sintered porous stainless steel and the cathode consists of carbon cloth. Bipolar plates separate the cells in the stack, ensures electrical conduction between the cells and distribution of the reacting agents. The used materials in the PEM electrolysis consist of a Nafion separation membrane, covered with a platinum coating of 0.75 mg/cm<sup>2</sup> and an iridium coating of 2 mg/cm<sup>2</sup> [67]. The cells in the PEM electrolysis have an additional layer to aid in the diffusion of the gasses.

After the formation of hydrogen and oxygen in the stack electrolyzer, a gas-liquid separator separates hydrogen and oxygen from water and other impurities. Heat exchangers maintain the optimal temperature of the system and removes generated heat. A compressor cools the hydrogen for storage and transportation [67].



**Figure 5.2:** Conceptual design for proton exchange membrane electrolysis. W = electric power input, Q = thermal power, or heat transfer

# 6 TECHNO-ECONOMIC ANALYSIS

To determine the economical feasibility of the chosen methods (Section 4.3), an economic evaluation was performed. This evaluation provides the minimum fuel selling prices (MFSP) for these two methods. The MFSP was calculated according to formulas described in Section 3.2. To calculate and fill in the formulas, certain parameters were required: the fixed capital, annual depreciation, fixed OPEX and the variable OPEX. These parameters and the MFSP are shown in Table 6.3, where the cost in USD per kg are portrayed. These results are further studied in the sensitivity analysis; where the uncertainty of various parameters are discussed.

### 6.1 ECONOMIC RESULTS

The fixed capital was calculated by using a Lang factor of 5.93 [52] and the total equipment cost. The total equipment costs are taken over a period of 20 years and are displayed in Table 6.1 and Table 6.2. The equipment cost for AE results in \$14.6 million and the PEM equipment cost results in \$10.5 million; the cost for both electrolyzers was based on Saba et al. [49]. The lifetime of both electrolyzers is considered to be 10 years, so two electrolyzers are required per method over a period of 20 years. The equipment cost of the rest of the equipment was based on the findings in Coulson & Richardson's Chemical Engineering Vol. 6 [1] and matche.com [48].

As shown in Table 6.3, the fixed capital for the PEM electrolysis is lower compared to the fixed capital of the AE. Certain parameters like the depreciation, fixed operating cost and partly the variable operating cost are dependent on the fixed capital. Besides the fixed capital, the variable OPEX is also dependent on the electricity usage (\$80/MWh) in the system (see utilities in Table 6.3). For this study, onshore wind electricity was chosen as the energy source. Overall, a higher MFSP is shown for the AE method compared to the PEM.

The required amount of iridium is dependent on the degradation of the catalyst and the total active area of the cell that is covered with the catalyst. It is known that under current conditions, iridium has a relatively high degradation rate; resulting in an annual required replacement of this catalyst [67; 71]. In the case of an annual replacement, an annual amount of 1.1 kg platinum (\$28,400 per kg) and 3.0 kg iridium (\$160,750/kg) is required [72] for an active area of 0.1 m<sup>2</sup> of 1,500 cells [67].

The variable operational expenses show values of \$5.23 and \$5.59 per kg H2 for AE and PEM. The cost contributions of the raw material (water) and utilities (platinum, iridium and electricity) are in more detail shown in Figure 6.1. This figure shows that the foremost contribution for the variable OPEX comes from the electricity usage. Another relatively high contribution is the usage for the platinum and iridium catalyst and the usage of the miscellaneous materials (plant supplies, required to operate the plant) [1]. Other contributions such as water, KOH solution the iron coating are low and in this case, negligible compared to the other cost contributions.

Equipment	n	Cost (\$)	Total cost (\$)
Alkaline electrolyzer	2	6,250,000	12,500,000
Heat exchanger	4	400,000	1,600,000
Ion exchange	1	300,000	300,00
G/L separator	2	13,000	26,000
Condenser	2	10,000	20,000
Pumps	4	42,000	168,000
Total			14,627,000

 Table 6.1: Equipment cost alkaline electrolysis

Table 6.2: Equipment cost proton exchange membrane	e electrolysis
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Equipment	n	Cost (\$)	Total cost (\$)
PEM electrolyzer	2	4,200,000	8,400,000
Heat exchanger	4	400,000	1,600,000
Ion exchange	1	300,000	300,00
G/L separator	2	13,000	26,000
Condenser	2	10,000	20,000
Pumps	4	42,000	168,000
Total			10,514,000

### 6.2 SENSITIVITY ANALYSIS

The minimum fuel selling price (MFSP) in the base case for AE is \$21.46, as shown in Table 6.3. Figure 6.2 shows the influence of the (a) equipment cost, (b) interest rate and (c) price of electricity on the total production cost of hydrogen per kilogram. The equipment cost affects directly the depreciation cost and thus of influence of the MFSP. A variation of equipment cost of  $\pm$  30% leads to a difference in MFSP of about \$3.79/kg. A deviation of the interest rate would affect the depreciation directly and changes the MFSP. A change in interest rate by  $\pm$  5% changes the production price by \$3.27 - \$3.72.

The electricity price during this study was established to be 80/MWh. However, the price of electricity fluctuates over the year. Therefore the price variation was set on 60-100 MWh [73]. This difference in electricity price leads to a variation in the MFSP of  $\pm$  \$1.08 per kg hydrogen.

As already shown in Table 6.3, the MFSP in the base case for PEM is \$17.40. The sensitivity analysis for the PEM electrolysis (Figure 6.3) was performed on a similar way as for the AE, with the addition of the active surface area of the cell and the replacement time of the catalyst (in years). The change in total active area was set to be  $\pm$ 50%. The replacement time was set on a varying time period from 1-10 years. These results, including the sensitivity of the equipment cost, interest and electricity are shown in Figure 6.3.

The variation of 30% in equipment prices would lead to a change the MFSP by  $\pm$  \$2.73 per kg hydrogen. A 5% change in the interest rate would lead to a MFSP

	AE	PEM
Fixed capital (M\$)	86.76	62.32
Unit costs (\$/kg H2)		
Depreciation	10.19	7.32
Fixed OPEX	1.42	1.02
Variable OPEX	5.48	5.59
- Raw materials	0.01	0.01
- Utilities	4.35	4.95
- Nafion	0.00	0.02
- Platinum catalyst	0.00	0.03
- Iridium catalyst	0.00	0.55
- Electricity	4.35	4.35
- Miscellaneous materials	0.87	0.63
Additional OPEX	1.33	1.13
Total production cost	17.16	14.05
MFSP	21.46	17.56

 

 Table 6.3: Minimum fuel selling price (MFSP) and cost contributions of the hydrogen production processes. OPEX denotes operational expenditures, electricity accounts only for electrolysis stack.



Figure 6.1: Cost contributions of raw materials and utilities for the variable OPEX



**Figure 6.2:** Sensitivity of MFSP Alkaline Electrolysis to economic parameters. MFSP in the base case is \$21.46. The sensitivity analysis shows the effects of a)  $\pm$ 30% (\$4.40M) change of the equipment cost, b)  $\pm$ 5% change interest rate, c)  $\pm$ \$20/MWh change electricity cost.

change of \$2.36 - \$2.69. The difference in electricity prices of \$60-100 MWh leads to a MFSP change of \$1.08 per kg hydrogen.

The assumption used for the base case was that the catalyst should be annually replaced. The sensitivity analysis analyzed the effect of a replacement over a longer period of time. If this replacement time would be 10 years, the MFSP would decrease with 0.53/kg. Considering the degradation of the catalysts; in the base case the catalyst is annually replaced. If the catalyst would be replaced after a longer period of time, eventually being 10 years, would decrease the price by 0.53/kg. When the system requires  $\pm 50\%$  of the active surface area compared to the base case (and thus a lower amount of catalyst), this leads to a change in the selling price of 0.29/kg.



**Figure 6.3:** Sensitivity of MFSP PEM Electrolysis to economic parameters. MFSP in the base case is \$17.56. The sensitivity analysis shows the effects of  $\pm$ 30% (\$3.16M) change of the equipment cost,  $\pm$ 5% change interest rate,  $\pm$ \$20/MWh change electricity cost,  $\pm$  0.05 m<sup>2</sup>/cell, catalyst replacement every 1-10 years.

### 6.3 DISCUSSION

In the techno-economic analysis, the MSFP is used as indicator for the evaluation of the AE and PEM electrolysis methods. This section discusses the results presented in the Section 6.1 and Section 6.2.

To put the results of the techno-economic analysis into perspective, a comparison with other studies can be applied. The first comparison is applied to the study done by Bunse [47]; a study that this thesis used as guideline. The study done by Bunse [47] provided an economic evaluation of hydrogen production, even though this was done by another method and other feedstock. His conceptual design was based on a microbial electrolysis, using glucose, acetic acid and propanoic acid as feedstock, where in this study water was used as feedstock for a non-microbial based electrolysis.

Both Bunse and this study used the MFSP to indicate the financial suitability of each method. The annual depreciation, fixed OPEX, variable OPEX and additional OPEX sum up the total production cost, on which the MFSP is based on; as is shown in Table 6.3. The MFSP in the study by Bunse resulted in a range of \$15.21-\$19.74, which is similar to the results in this study (\$17.55 - \$21.46). In Bunse's study, the major costs come from the raw materials, whereas in this study, the cost of feed-stock are low. The difference in raw material cost can be explained due to the fact that this study utilizes water as feedstock, which is lower in cost compared to a saccharide based feedstock in the study by Bunse.

The biggest contribution to the MFSP for this study is provided by the annual depreciation; \$10.19 for AE and \$7.32 for the PEM. The annual depreciation is determined by two parameters: the interest rate and the total equipment cost. The interest rate was set at 10%, the same as similar study by Bunse [47], using Coulson et al. [1] as a guideline. The fixed capital in the study of Bunse [47] varied from \$81.5 M to \$127.1 M, which are similar values compared to the fixed capital of this study; \$62.3 M - \$86.85 M. However, the annual depreciation cost are 5-10 times higher for this study, compared to the \$1.00 - 1.43 per kg hydrogen in the study of Bunse [47]. An explanation for the difference in annual depreciation might be caused by a difference in production quantity. The production capacity in this

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study was set at one million kilogram of hydrogen; to the authors knowledge, it is not clearly stated in Bunses research. On the other hand, the results for the fixed capital and annual depreciation are similar to comparable studies like Wei et al. [74]. Wei et al. provided a study on the techno-economical assessment on PEM electrolysis, where capital cost were \$113M - \$130M and an annual capital repayment of \$8M - \$9M, which is similar to this study.

The contribution of the fixed OPEX to the MFSP is relatively lower than that of the annual depreciation. These costs are directly connected to the value of the fixed capital; costs like maintenance and operating labour. The total value for the fixed operating cost is divided by the lifetime of the plant, which is 20 years. Resulting in an annual fixed OPEX of \$1.0 - \$1.4 million. These costs are considered to be low, compared to other work. Bunse [47] showed a variable OPEX of \$2.5 - \$3.0 per kg.

The variable OPEX has a significant contribution to the MFSP Figure 6.1. This high contribution is caused by the electricity cost for the electrolysis methods. The utility cost for the PEM electrolysis was also influenced by the use of catalysts; iridium and platinum. With a kilo price of \$160,750 and \$26,400 [72] respectively, these catalysts have a significant influence on the MFSP. The active surface area, number of cells and the thickness of the coating layer all influence the cost of these catalysts. Based on an annual production of 1 million kg hydrogen for the base case, \$500,000 worth of iridium and \$32,000 worth of platinum would be required [67; 71]. However, this might range from \$250,000-\$750,000 worth of iridium and \$16,000-\$48,000 worth of platinum for a  $\pm$  50% change in active surface.

In addition to that, it is known that under current conditions, iridium has a relatively high degradation rate; resulting in an annual required replacement of this catalyst [67; 71]. The platinum catalyst on the other hand is more robust. Research is being done to increase the recycling rates of the iridium. These recycling rates show results from 40% to 90% [71]. This would lead to a delay of the replacement time for the iridium.

Other studies and sources present lower production costs for the hydrogen production. in the study from Groenemans et al. [75], it is presented that a hydrogen price of \$2 - \$3 per kg should be possible; a selling price that is considerably lower compared to the findings in this study. One reason for this gap is that the results in the study performed by Groenemans et al. [75] was designed for a 3.1 GW plant, while the plant in this study was designed for 6.67 MW. Currently, the up-scaling for the PEM electrolysis is still in development [76], so calculations for a 3.1 GW plant are an interesting view for the future, but optimistic for the current situation. Hande [77] presents that the production cost of hydrogen can be in the range of \$4 -\$5 per kg, which is similar to the variable cost in this study (approximately \$5.50 for both AE and PEM). A production cost of \$4 - \$5 per kg might be true, when only referring to the variable operating cost. However, presenting just the production cost gives an incomplete view on the selling price, which also includes the fixed cost, annual depreciation cost and a profit margin.

The sensitivity analysis shows how sensitive these methods are when adjusting certain parameters. As can be seen in Figure 6.2, the equipment cost are of big influence to the MFSP; this indicates that when the price for equipment goes down, it would have a big effect on the selling price. A lower interest rate would also lead to a significantly lower price; the annual depreciation is directly linked to the interest rate and a change of couple percentages would lead to a lower price. Given the results shown in Figure 6.1, where the electricity contribution to the variable OPEX was the biggest contribution, a significant effect on the MFSP was expected. Although the effect of the lower electricity price per MWh is noticeable, it is also

not significantly big. This can be explained by the fact that the contribution of the variable OPEX is smaller compared to the depreciation, which is linked to both the equipment cost and the interest rate. Therefore the effect of the former two parameters are bigger compared to the electricity price. In the most favourable situation, with a lower equipment cost, interest rate and electricity price would save about \$8/kg hydrogen. When the results of sensitivity analysis in the most favourable situation would be applied, a selling price of \$12.63 and \$9.77 per kg would arise for AE and PEM electrolysis respectively. Technological improvements and beneficial economic circumstances would lead to a decreasing MFSP. Another way to keep the price down is producing on bigger scale; this study looked at a production of 1 million kg hydrogen per year, but for future references the production scale could increase, which lowers the fixed costs per kg.

## 7 CONCLUSION AND OUTLOOK

### 7.1 CONCLUSION

This work presents a techno-economic analysis on (bio)electrochemical methods for the production of hydrogen. Six methods were selected to be analyzed by an early stage analysis, which provided an exploratory screening to choose from literature. The two best scoring methods were further conceptually designed and a techno-economic evaluation was performed. Thereafter, the sensitivities of the early-stage analysis and the techno-economic evaluation were determined and further discussed.

The early stage analysis was performed from both an economic and environmental view. Based on these results and the technological maturity, two methods were selected for further analysis in the techno-economic evaluation; the alkaline electrolysis (AE) and proton exchange membrane (PEM) electrolysis. A sensitivity analysis was applied on the parameters in the early stage analysis, with the economic constraint parameter as the most significant and influential. The sensitivity analysis showed no big variations for the AE and PEM electrolysis, and could therefore be determined as stable methods. After determining the most promising methods, the research question was studied; which is to identify sustainable hydrogen production methods that could be used for large-scale production, their cost contributions and how variations in key parameters impact the overall production costs.

To answer these questions, a concept process was designed for both methods for an annual production of 1 million kg hydrogen. For AE, a stack of 700 cells with an area of 2.1 m<sup>2</sup> was considered for the electrolysis using water and KOH as electrolyte, with a power input of 50 kWh. The techno-economic analysis assessed the fixed cost, variable cost and additional cost, resulting in a total production cost of \$17.16 and an MFSP of \$21.46. For PEM electrolysis, a stack of 1,500 cells with an area of 0.1 m<sup>2</sup> was used in the concept design; also with power input of 50 kWh. The total active area is covered with a thin layer of platinum or iridium, used as catalyst. In the base case, an annual replenishment of 1.1 kg platinum (\$28,400 per kg) and 3.0 kg iridium (\$160,750/kg) would be required. The techno-economic analysis for PEM resulted in a total production cost of \$14.05 and a MFSP of \$17.56. For both cases, the biggest cost contributions were the annual depreciation and the electricity cost.

The highest contributions to the MFSP was the depreciation. The depreciation in this study resulted in \$7.32 - \$10.19 per kg hydrogen, although these values for depreciation are similar to the work of Wei et al. [74]. Compared to other sources, the selling prices presented in this thesis were higher. Groenemans et al [75] presented a price of \$2 - \$3 per kg, however, his calculations were based on a 3.1 GW plant, so the scaling-up lowers the selling price per kg. Another source was Hande [77], where only the variable production cost were shown, which was \$4 - \$5. This value was similar to the variable production cost in this study, which was around \$5.50 for both AE and PEM.

The techno-economic and sensitivity analyses on both AE and PEM electrolysis, identified PEM electrolysis as the superior method, achieving a minimum fuel selling price (MFSP) of \$17.56, compared to \$21.46 for AE. The depreciation was identified as the biggest contributor to the MFSP; being \$10.19/kg for AE and \$7.32/kg for PEM. The sensitivity analysis showed the biggest variations by changing the equipment cost and the interest rate. Especially technological improvements on the equipment would lead to a decreasing MFSP; a decrease of 30% in equipment cost would lead to -\$3.79 for AE and -\$2.73 for PEM.

### 7.2 OUTLOOK

Electrolysis for hydrogen production is a growing field, where it is expected that within a few years the first 100 MW plants will be put in use. Big scale production will decrease the fixed cost per produced kg hydrogen and eventually lead to the variable cost being the main cost contributor. Current challenges involve generating affordable and sustainable electricity, which significantly impacts variable costs. Also, technological improvement in the production and equipment would lead to better scaling-up possibilities and thus lowering the fixed cost for the equipment. It is recommended to apply a study on the scaling up of the AE and PEM electrolysis.

For another recommended follow-up study, it would be advised to study the solid oxide electrolyzer cell (SOEC). SOECs are considered highly efficient for hydrogen production; however, they are currently less mature and face challenges in scalability. Finally, this study mainly focused on the techno-economic aspects of the electrolysis methods. It is recommended that future research also include an environmental impact assessment.

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APPENDIX



#### **RESULTS SENSITIVITY ANALYSIS** A.1



(a) CED sensitivity on aggregated process scores



(c) CED + GWP sensitivity on aggregated process scores

Figure A.1: Sensitivity of 50 % up- and downregulated (a) CED values, (b) global warming potentials and (c) combined CED and GWP on the early stage analysis process scores of hydrogen production

