Techno-economic evaluation of the hybrid sulphur chemical water splitting (HyS) process

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Innovation through diversity

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ABSTRACT

The constantly growing demand for energy and the consequent depletion of fossil fuels have led to a drive for energy that is environmentally friendly, efficient and sustainable. A viable source with the most potential of adhering to the criteria is nuclear-produced hydrogen. The hybrid sulphur cycle (HyS) is the proposed electro-thermochemical process that can produce the energy carrier, hydrogen. The HyS consists of two unit operations, namely the electrolyzer and the decomposition reactor, that decomposes water into hydrogen and oxygen. A techno-economic evaluation of the technology is needed to prove the commercial potential of the cycle. This research project focuses on determining the hybrid sulphur cycle's recommended operating parameter range that will support economic viability whilst maintaining a high efficiency. This is done by comparing the results of an evaluation of four case studies, all operating under different conditions.

The technical evaluation of the research project is executed using the engineering tool Aspen Plus^{TM}. The models used to achieve accurate results were OLI Mixed Solvent Electrolyte, oleum data package for use with Aspen Plus^{TM}, which provides an accurate representation of the H_2SO_4 properties, and ELECNRTL to provide an accurate representation of H_2SO_4 at high temperature conditions. This evaluation provides insight into the efficiency of the process as well as the operating conditions that deliver the highest efficiency. The economic evaluation of the research project determines the hydrogen production costs for various operating conditions. These evaluations provide a recommended operating parameter range for the HyS to obtain high efficiency and economic viability.

Keywords: Hydrogen, Hybrid Sulphur, Techno-economic, Nuclear-produced, Process simulation

OPSOMMING

Die vraag na energie het in die laaste dekades gegroei terwyl fossielbrandstowwe uitgeput word. Daar is dus'n behoefte aan 'n omgewingsvriendelike, effektiewe en volhoubare energiebron. Die bron wat geïdentifiseer is as die een met die grootste potensiaal wat aan dié vereistes voldoen, is waterstof wat vervaardig word deur kern-energie. Die hibried swael siklus (HyS) is die voorgestelde elektro-termiese proses wat hierdie waterstof kan vervaardig. Die hibried swael proses maak gebruik van twee proseseenhede, naamlik die elektroliseerder en die chemiese-ontbindings reaktor, om water te ontbind in waterstof en suurstof. 'n Tegno-ekonomiese evaluasie van die tegnologie word benodig om die kommersiële lewensvatbaarheid van die siklus te bewys. Die navorsingsprojek fokus op die bepaling van die Hys se bedryfsparameters sodat ekonomiese lewensvatbaarheid sowel as termiese doeltreffendheid verseker word. Dit word gedoen deur die evaluering van resultate van vier gevallestudies, wat bedryf word onder verskillende operasionele omstandighede.

Die tegniese evaluasie van die navorsingsprojek word uitgevoer deur gebruik te maak van die ingenieurssimulasie program Aspen Plus^{TM}. Die eienskap-model vir H_2SO_4 wat binne Aspen Plus^{TM} gekies is, is die *OLI Mixed Solvent Electrolyte,* oleum data pakket vir gebruik met Aspen Plus^{TM}. Daar is ook gebruik gemaak van die *ELECNRTL* eienskap-model vir akkurate resultate by hoë temperature vir H_2SO_4. Die navorsingsprojek gee beter insig oor die termiese doeltreffendheid van die proses asook die bedryfskondisies wat hoë doeltreffendheid verseker. Die ekonomiese evaluasie van die proses bepaal die waterstof produksiekostes vir 'n verskeidenheid bedryfskondisies. Die resultate bepaal die voorgestelde bedryfskondisies vir die hibried swael proses om hoë termiese doeltreffendheid sowel as ekonomiese lewensvatbaarheid te bereik.

Sleutelterme: Waterstof, Hibried Swael, Tegno-ekonomiese, Kern-energie, Proses simulasie

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ABBREVIATIONS

This list contains the abbreviations as used in this research project.

Abbreviation	***Term***
BOP	Balance of Plant
CAPEX	Capital Expenditure
CEPCI	Chemical Engineering Plant Cost Index
FACES	Factored Automated Cost Estimating System
FCI	Fixed Capital Investment
GGE	Gallons of Gas Equivalent
GHG	Greenhouse Gases
GTMHR	Gas Turbine Modular Helium Reactors
HHV	Higher Heating Value
HPS	Hydrogen Processing System
HTSE	High Temperature Steam Electrolysis
HyS	Hybrid Sulphur Cycle
IRR	Internal Rate of Return
LHV	Lower Heating Value
MMBtu	Million British Thermal Unit
MSE	Mixed Solvent Electrolyte
Mtoe	Million tons of oil equivalent
MWh	Megawatt hour
NHSS	Nuclear Heat Supply System
Non-OECD	Non-Organization for Economic Co-operation and Development
OECD	Organization for Economic Co-operation and Development
OPEX	Operating Expenditure
PBMR	Pebble Bed Modular Reactor
PEM	Proton Exchange Membrane
PGS	Power Generating System
SDE	SO_2-Depolarized Electrolyzer
SI	Sulphur Iodine Cycle
SMR	Steam Methane Reforming
SRNL	Savannah River National Research Laboratories
TCI	Total Capital Investment
TPD	Tons Per Day
VHTR	Very High Temperature Reactor
WCI	Working Capital Investment
MWt	Megawatt thermal
wt%	Weight percentage
MT	Million tons
kg	Kilogram
s	Second
$	United States Dollar
H_2SO_4	Sulphuric acid
SO_2	Sulphur dioxide
SO_3	Sulphur trioxide
O_2	Oxygen
H_2O	Water
HI	Hydrogen Iodine

He	Helium
kJ/g	Kilojoules per gram
GJ	Giga joules
ºC	Degree Celsius
K	Degree Kelvin
MW	Megawatt
kmol	Kilomol
kJ	Kilojoules
mol%	Mol percentage
mA/cm^2	Milliampere per centimeter squared
bar	Pressure in bar units
RO/EDI	Reverse osmosis / Electro-Deionization

CHAPTER 1

INTRODUCTION

1. Introduction

The global energy sector is currently confronted with an energy crisis. This crisis involves a significant increase in energy demand and consumption whilst facing a depletion of non-renewable energy sources (Midilli & Dincer, 2008:4209). The energy sector is also confronted with the concern of non-renewable energy's effect on the environment and is largely blamed for global warming and climate change. The supply shortage and environmental concerns has lead to international regulations on greenhouse gas emissions in the form of the Kyoto Protocol. This chain of events gave momentum to the search for an alternative energy source. Such an alternative source must consist of the following factors (Balat, 2008:4014):

- Technical feasibility and proven technology.
- Energy efficient production process.
- Sustainability.
- Economical feasibility and competitiveness.
- Clean and environmentally friendly.

The purpose of this study is therefore to investigate the technical and economical aspects of the Hybrid Sulphur Cycle (HyS) and to determine whether this process could potentially be applied as a viable alternative source of energy.

1.1 Global energy scenario

The world is entering a period of shortage in energy, electricity, petroleum and oil. According to the International Energy Outlook 2008 (IEO, 2009), the world energy demand will increase by 45% between 2008 and 2030. This implies an average increase rate of 1.6% in the global energy demand per year. Coal will be responsible for more than a third of the overall increase in energy consumption. The world energy consumption totalled to 135×10^9 MWh (Megawatt hour) in 2005 and is estimated to grow to 203×10^9 MWh by 2030 (IEO, 2009). This is expected despite projected long term high oil prices. Figure 1 illustrates the historic and projected global energy consumption.

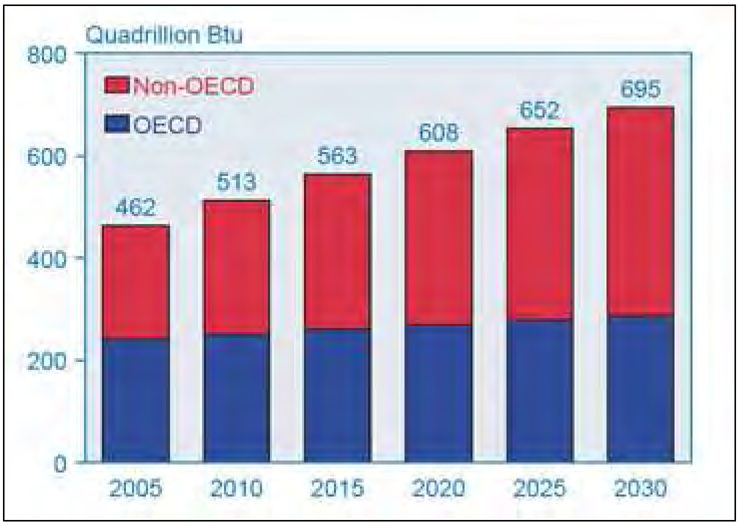

Figure 1: World energy consumption 2005-2030 (IEO, 2009).

There is a projected 85% increase (IEO, 2009) in energy consumption by non-OECD countries due to industrial growth and various social reasons and a 19% projected growth increase by developed countries.

Figure 2 illustrates the world's primary energy demand in the current (2008) available fuels (Mtoe – **M**illion **t**ons of **o**il **e**quivalent).

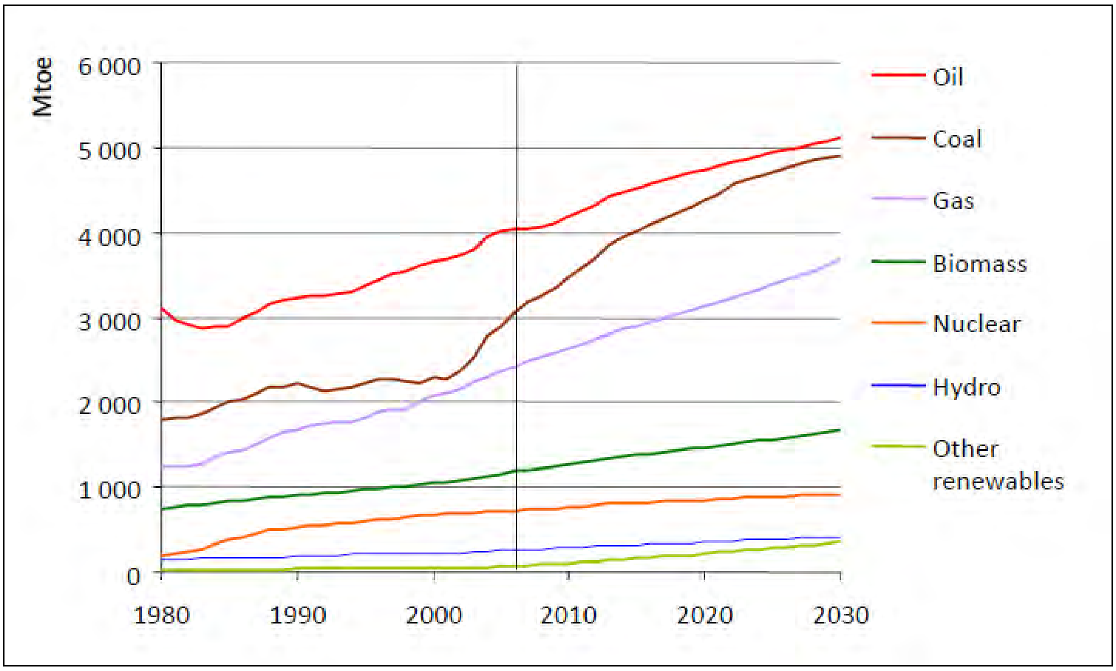

Figure 2: World primary energy demand (WEO: 2008).

As is evident from Figure 2, there is an increasing demand for energy due to the world population growth and the need of developing countries to provide economic and social wellbeing to its citizens. The consequence of the increasing energy consumption is the release of more greenhouse gases. Figure 3 illustrates energy related CO_2 emissions (IEO, 2009).

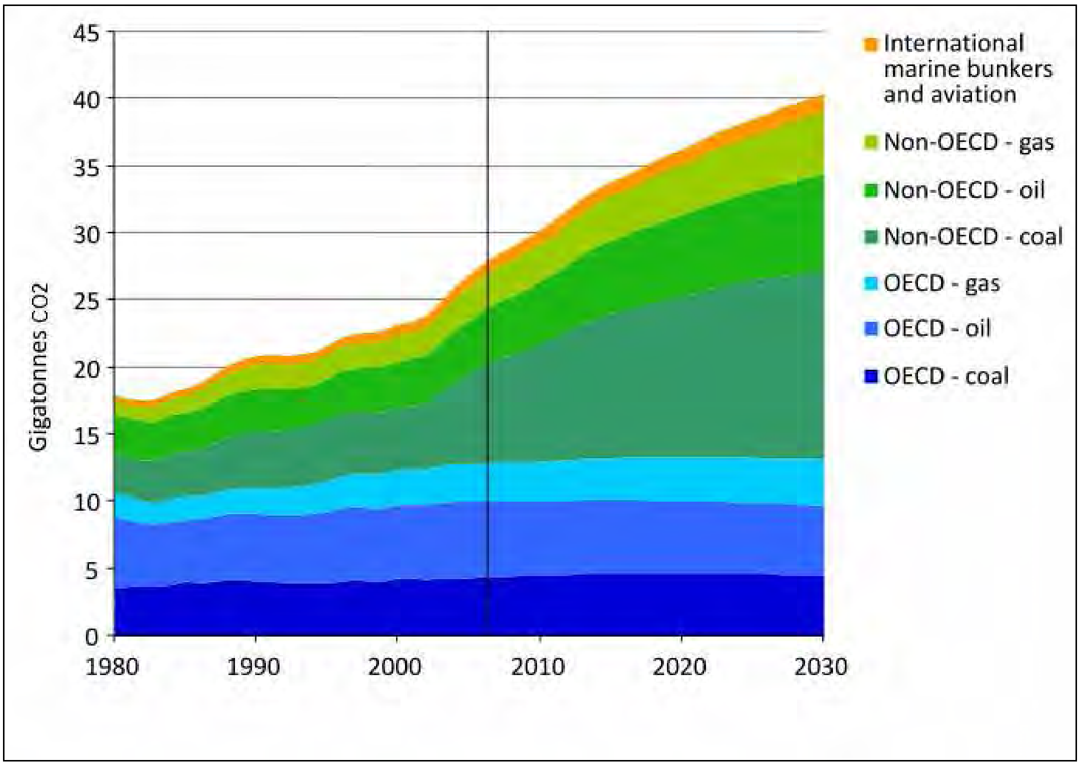

Figure 3: Energy-related CO_2 emissions (IEO, 2009).

A total of 28 gigatonnes of carbon dioxide (energy related) were released in 2002 and will increase to a projected 42 gigatonnes by 2030, if no alternative energy sources are developed. It is projected that India, China and the Middle East will be responsible for three quarters of the Non-OECD countries' emissions. As can be seen in Figure 3, coal is the largest contributor to CO_2 emissions.

This background knowledge of increasing energy consumption and demand together with the high pollution factor will highlight the disadvantages of fossil fuels. Fossil fuels are a limited energy source. Fossil fuels emit greenhouse gases that add to the global warming effect. The mining and processing phases of fossil fuels also cause pollution.

Scientists believe the increase in greenhouse gas emissions into the atmosphere is causing a climate change and global warming effect. Global warming is the increase of greenhouse gases in the atmosphere leading to the increase of the earth's near surface air temperature and that of the oceans. To mitigate global warming, the Kyoto Protocol was signed and ratified by most developed countries, thereby committing themselves to the reduction of greenhouse gas emissions.

1.2 Alternative fuels

Numerous potential alternative fuels have been identified, namely biofuels (methanol, ethanol and biodiesel), nuclear hydrogen, non-fossil natural gas, biomass and vegetable oil. In order to develop these alternative fuels, some factors must be kept in mind (Brey *et al.*, 1999:3):

- The most appropriate energy source must be identified.
- The technology must be efficient.
- The storage and transport methods of the fuel must be investigated.

Hydrogen is an alternative fuel that could potentially become the fuel of the future if the energy used to produce hydrogen causes less pollution than fossil fuel power. Hydrogen is a potential energy carrier and not an energy source. It therefore needs a primary energy source for production (Zerta *et al.*, 2008:3023). One such alternative power production method is nuclear power. Nuclear power is already produced at large scale and the next generation reactor designs have contributed to make nuclear power inherently safe. Nuclear power will assist to limit greenhouse gas emissions by electricity generating facilities.

1.3 Hydrogen economy

The global energy crisis has launched the birth of the hydrogen economy. It is envisioned that hydrogen will become the future energy carrier to replace fossil fuels as a major renewable energy source.

There are various possible methods of producing hydrogen, including steam methane reforming, partial oxidation of methane, coal gasification, biomass pyrolysis, hybrid sulphur cycle, high temperature steam electrolysis (HTSE) and the sulphur iodine cycle (SI). However, hydrogen is currently produced mainly from fossil fuels through natural gas reforming or gasification of coal processes. These processes emit carbon dioxide into the atmosphere, thereby adding to the energy related CO_2 emissions. Environmentally friendly methods and sustainable resources must be used in order for a hydrogen energy carrier to be considered as a renewable energy source with no harmful effects.

This mini-dissertation will focus on the hybrid sulphur cycle (HyS) for hydrogen production. The HyS is an electro-thermochemical decomposition cycle which firstly decomposes sulphuric acid (H_2SO_4) into water (H_2O), sulphur dioxide (SO_2) and oxygen (O_2) and then electrolyzes water and sulphur dioxide (SO_2) to produce hydrogen (H_2) and sulphuric acid. The net reaction is the dissociation of water into hydrogen and oxygen. The HyS is an environmentally friendly method that uses sustainable resources. Therefore the HyS cycle allows the hydrogen economy to be a promising future energy carrier.

The use of nuclear power for the production of hydrogen makes the case for hydrogen an even stronger candidate as an environmentally friendly energy carrier. Nuclear technology has developed advanced nuclear plant designs that can supply high temperature heat for hydrogen production. Such designs are helium cooled graphite moderated reactors (HTGR) and Pebble Bed Modular Reactors for example. These are third generation nuclear plant designs and are inherently safe, which makes the case even stronger for using hydrogen coupled with nuclear power.

Given that the HyS technology is environmentally friendly, a techno-economic evaluation of the cycle is required in order to establish and understand the technology and its efficiency and whether the technology is economically feasible. Previous studies have shown that the HyS hydrogen production thermal efficiency ranges between 35% - 48%. An optimization of the HyS study proposes a high temperature range (870ºC – 900ºC) and low operating pressure conditions (3 bar – 4 bar). Economic evaluations indicate a total direct depreciable cost for the PBMR HyS water splitting plant at 500 MWt and 160.1 TPD hydrogen production to be $1,108 million (Gorensek *et al.*, 2009:72). For the Hydrogen Processing System (HPS) the capital expenditure was estimated at $460 million, the Nuclear Heat Supply System (NHSS) at $450 million, the Power Generating System (PGS) at $57million and the Balance of Plant (BOP) at $147 million (Gorensek *et al.*, 2009:72). This mini-dissertation will determine the relation between the optimal operating point and the economic implications thereof, by determining the economic viability of the HyS process based on the calculated technical data (Gorensek *et al.*, 2009:72).

1.4 Background

Hydrogen is the most abundant element on earth but exists as a chemical compound and not as pure hydrogen. It occurs naturally in fossil fuels, water and most organic compounds. Hydrogen has a greater energy yield (122 kJ/g) than other hydrocarbon fuels and higher specific energy content than conventional fuels (Energy density of 143 kJ/kg). Hydrogen is mainly used in the production of ammonia (49%), petroleum refineries (37%), methanol production (8%) and other miscellaneous uses (6%). The global hydrogen market worth is $40 billion per year (Balat, 2008:4014).

The transport sector developed technology that uses hydrogen as a fuel in combustion engines and fuel-cell electric vehicles. Hydrogen as a transportation fuel is very efficient and produces non-toxic exhaust emissions in the form of water vapour.

1.5 Problem Statement

There has been a large drive for cleaner energy for decades. The high oil and energy prices and high carbon dioxide emission levels generated by fossil fuels intensified this pursuit. To find a new energy source that is environmentally friendly, efficient and sustainable is imperative. The hybrid sulphur cycle is an electro-thermochemical process that produces hydrogen, a future energy carrier. To achieve a successful industrial process, a techno-economic evaluation is needed to prove the technology readiness and the commercial potential of the cycle. This mini-dissertation will focus on determining the hybrid sulphur cycle’s recommended operating parameter range that will support economic viability with the highest energy efficiency.

1.6 Research Methodology

A techno-economic evaluation of the hybrid sulphur cycle consists of two individual evaluations followed by a modelling process to relate the two evaluations.

The methodology used for this research will start with an initial literature survey on the current energy usage and availability. Information on technical evaluations done on the HyS will be gathered. This will include topics such as optimization studies, cycle efficiency, temperature, pressure, acid concentration and product yield. Information on economic evaluation done on the HyS will also be gathered. The topic will include capital expenses (CAPEX), operating expenses (OPEX), hydrogen costs, etc.

After completing the literature survey and gathering all information necessary for developing a flowsheet and economic model, the simulation of the cycle will be carried out. A flowsheet will be developed and solved making use of the simulation package Aspen Plus™. This simulation package is a process modelling tool for conceptual designs, optimization and performance monitoring of chemical processes. The hydrogen and oxygen production rates for the corresponding operational conditions will be determined using Aspen Plus™.

The completion of the flowsheet simulation will be followed by the development of an economic model that will include the CAPEX and OPEX of the process. The model will be developed in Microsoft Excel ©.

The final step will include the process of relating the technical evaluation to the economic evaluation. For each simulation of a specific operational condition, the corresponding CAPEX and OPEX in the economic model will be determined. The input values and output values from the simulation of the corresponding operational conditions will be fed into the economic results MS Excel model, that will determine the cost of hydrogen production for each case.

1.7 Focus of this study

The aim of this study is to investigate the hybrid sulphur cycle for hydrogen production. The mini-dissertation will focus on the following in order to arrive at a conclusion:

- Develop a flowsheet of the HyS process using an engineering simulation package. The proposed package to be used is Aspen Plus^{TM}.
- Perform a technical evaluation of the process by determining the operational conditions (minimum and maximum) that will deliver the optimal and worst case process thermal efficiency. Variable factors included are sulphur trioxide (SO_3) reactor temperature, sulphur trioxide reactor pressure, electrolyzer acid concentration and the concentrator's acid concentration.
- Calculate the hydrogen and oxygen production rates of the corresponding operational conditions under investigation.
- Determine the capital expenditure (CAPEX) of the process.
- Determine the operating expenditure (OPEX) of the process.
- Discuss the details of the pressure and temperature effects on capital costs or feasibility of the process. Conduct a sensitivity analysis on the process to determine the economic implications on the evaluated process conditions.
- Design an economic model to determine the proposed hydrogen production price ($/kg) of the proposed hybrid sulphur plant. This includes the hydrogen production cost, oxygen cost, variable and fixed costs.
- Determine the recommended operating parameter range of the HyS process to sustain economic viability.

1.8 Outline of mini-dissertation

The mini-dissertation is outlined as follows:

- Chapter 1 gives a basic introduction on the global energy crisis and possible solutions to the problem. The concept of a hydrogen economy is introduced together with some general facts about hydrogen. The mini-dissertation problem statement is also given in this chapter.
- Chapter 2 offers an investigation into the hydrogen economy, the methods used to produce hydrogen and some technical and economical evaluations done on hydrogen production methods.
- Chapter 3 describes the proposed hybrid sulphur cycle in detail including the software packages used to perform the analysis.
- Chapter 4 provides the proposed flowsheet of the hybrid sulphur cycle and the results from the technical evaluation of the cycle.
- Chapter 5 reports on the capital and operating expenditure of the HyS which the economic model is based on, with its technical specifications. The chapter further also evaluates the implications of the operational conditions on the economic model.
- Chapter 6 explains the results obtained from the techno-economic evaluation.
- Chapter 7 offers conclusions and recommendations for the HyS technology and suggestions for future research to be done.

CHAPTER 2

LITERATURE STUDY

2. Literature Study

2.1. Introduction

Chapter 1 gave a basic introduction into the extent of the energy problem that the world is facing and the potential solution that could be found in the hydrogen research field, as a background description into the problem.

Chapter 2 will describe hydrogen production methods in detail, providing more background into the engineering problem. The efficiencies of the various methods will be given and some comparisons between the methods will be made. Previous studies done on the cost analysis of the HyS will also be discussed together with some comparisons between the methods.

2.2. Hydrogen Production Methods

The first method that will be discussed is the hydrogen production based on fossil fuels followed by the hydrogen production methods making use of nuclear process heat and alternative energy sources.

2.2.1 Steam Methane Reforming

The steam methane reforming process (SMR) uses methane as the feedstock and consists of three step reactions that ultimately produce hydrogen. The methane is reformed at high temperatures and pressures, in the presence of a catalyst, to produce a mixture of hydrogen and carbon monoxide. This mixture is also known as a syngas and contains carbon dioxide (CO_2) and other impurities. Carbon monoxide is then combined with water to produce hydrogen. Thereafter the hydrogen is submitted to a purification process to deliver the product at the desired product quality. The purification is done by means of adsorption (McHugh *et al.*, 2005:2-1).

The steam methane reforming is described by the following reactions (McHugh *et al.*, 2005:2-1):

$$CH_4 + H_2O \leftrightarrow 3H_2 + CO \qquad \Delta H = +206 \text{ kJ/mol} \qquad (1)$$

$$2CO \leftrightarrow CO_2 + C \qquad \Delta H = -172 \text{ kJ/mol} \qquad (2)$$

$CO + H_2O \leftrightarrow CO_2 + H_2$ $\Delta H = -41$ kJ/mol (3)

Reaction (1) describes the reforming step. This reaction is an endothermic reaction and takes place in a reformer that contains tubes filled with a nickel catalyst. Here the methane reacts with high temperature steam to produce hydrogen and carbon monoxide. The reaction conditions are at temperatures between 500℃ and 950℃ at pressures of up to 30 bar (McHugh *et al.*, 2005:2-1).

Sulphur is removed from the methane gas before it enters the tubes filled with the nickel catalyst by passing the methane gas through guard beds containing zinc oxide or activated carbon. This helps to prevent the deactivation of the nickel catalyst (McHugh *et al.*, 2005:2-1).

Reaction (2) is known as the nickel catalyzed Boudouard reaction that entails thermal cracking and coking. This is an exothermic reaction that could be prevented by means of achieving excess steam within the system. This in effect increases the conversion of syngas to hydrogen (McHugh *et al.*, 2005:2-1).

Reaction (3) is the step following methane reforming. This reaction is known as the "water gas shift". The reaction occurs in several stages at temperatures lower than the reforming reaction in the presence of a catalyst. The type of catalyst depends on the operating conditions. At higher temperatures (350℃) an iron based catalyst is used while at lower temperatures (205℃) a copper b ased catalyst is rather used (McHugh *et al.*, 2005:2-2).

The production of hydrogen is followed by a purification step. This is to achieve the desired product quality. This could be done by two possible methods namely pressure swing absorption or chemical absorption of hydrogen. A 99.99% pure hydrogen product can be produced using the SMR method.

The steam methane reforming process has an 83% thermal efficiency. This method is currently the most economic hydrogen production method with a hydrogen production cost of \$0.75/kg or \$5.25/GJ (assuming a natural gas price of \$2.99/GJ) (McHugh *et al.*, 2005:2-3). The gas price increased in the last few years and is now in the range of \$8/GJ - \$10/GJ.

Steam methane reforming is the process that is most widely used process when producing hydrogen. The process has a high efficiency, favourable economics and proven and established technology.

Other processes that make use of non-renewable energy sources are:

- Partial oxidation/autothermal reforming of methane.
- Coal gasification
- Biomass pyrolysis/gasification.

2.2.2 Electrolysis

Electrolysis is the process during which electricity is used to dissociate water into hydrogen and oxygen. The electricity generation could be from either renewable or non-renewable sources.

The dissociation of water by means of electrolysis is achieved by applying an electric potential across a cell. The cell consists of two electrodes, a cathode and anode, and a conducting medium such as an alkaline electrolyte solution. The conducting medium is an aqueous solution of potassium hydroxide (KOH) which helps to conduct electrons that are released and absorbed at the electrodes. For electrolysis, hydrogen is formed at the cathode and oxygen at the anode with water as the feedstock and electricity as the energy source (McHugh *et al.*, 2005:3-1).

The reactions for this process are given as follows (McHugh *et al.*, 2005:3-1):

Cathode: $2H_2O + 2e^- \rightarrow H_2 + 2OH^-$

Anode : $2OH^- \rightarrow ½\,O_2 + H_2O + 2e^-$

Net Reaction: $H_2O \rightarrow H_2 + ½\,O_2$

The reaction rate is determined by the voltage that is applied over the cells. The voltage theoretically required for this reaction to occur is 1.23V. Even at this voltage the reaction is slow and therefore a higher voltage is needed to increase the reaction rate, which in turn decreases the energy efficiency because of higher heat losses to the environment. Various methods are used to increase this efficiency. Some examples are increased temperature and pressure conditions for the electrolyzer made of higher costing material to resist corrosion and high pressure or simply by introducing a catalyst to the electrolyzer which could increase the reaction rate (McHugh *et al.*, 2005:3-1).

For the electrolysis process there are various types of electrolyzers that could be used. The three industrial types available are unipolar tank type, bipolar filter press and proton exchange membrane (PEM) electrolyzer. The PEM electrolyzer is different from the unipolar and bipolar electrolyzers as it does not use potassium hydroxide as an electrolyte. It does, however, have the same net reaction (McHugh *et al.*, 2005:3-2):

Cathode: $2H^+ + 2e^- \rightarrow H_2$

Anode: $H_2O \rightarrow \frac{1}{2} O_2 + 2H^+ + 2e^-$

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

The PEM electrolyzer uses a membrane as the electrolyte and only requires simple electrodes. The unipolar contains cathodes and anodes suspended in the electrolyte tank while the bipolar contains electrodes stacked closely together. Both these types have a membrane separating the cathodes and the anodes, thus preventing dissolved gases and bubbles from mixing.

The industrial electrolysis process for hydrogen production is proven technology with a process efficiency of 45-55%. The cost of producing hydrogen at high temperature electrolysis is \$13.74/GJ or \$1.95/kg hydrogen (McHugh *et al.*, 2005:3-4).

2.2.3 Sulphur Iodine Cycle

The sulphur iodine cycle (SI) is a thermo-chemical cycle that produces hydrogen and oxygen through the decomposition of water and the addition of heat. The SI process produces no harmful emissions or by-products. The process makes use of water as the feedstock and a heat source to drive three thermo-chemical reactions that includes sulphur and iodine. The heat source origin could possibly be from a nuclear gas-cooled reactor which provides process heat at 850℃ and 950℃. The chemical reactions that describe the process are as follows (McHugh *et al.*, 2005:3-7):

$I_2 + SO_2 + 2H_2O \leftrightarrow 2HI + H_2SO_4$	(<120℃)	$\Delta H = -216$ kJ/mol	(4)
$H_2SO_4 \leftrightarrow SO_2 + H_2O + \frac{1}{2} O_2$,	(>800℃)	$\Delta H = +371$ kJ/mol	(5)
$2HI \leftrightarrow H_2 + I_2$,	(>300℃)	$\Delta H = +12$ kJ/mol	(6)

The net reaction is:

$$H_2O \rightarrow H_2 + \frac{1}{2} O_2 \tag{7}$$

Reaction (4) is called the Bunsen-reaction and produces two immiscible aqueous products namely a light aqueous sulphuric acid and a heavy mixture of hydrogen iodide and iodine. These two products can easily be separated by gravity. In reaction (5) hydriodic acid (HI) is decomposed by means of reactive distillation and in reaction (6) sulphuric acid is decomposed by catalytic decomposition, concentration and vaporization. Figure 4 represents the SI reactions in a simplified flowsheet.

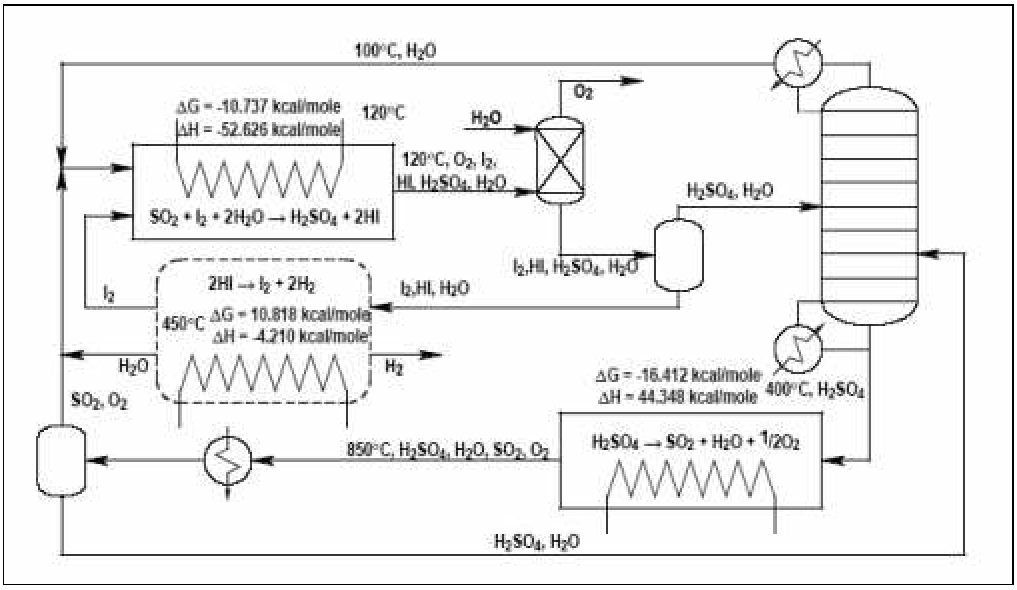

Figure 4: Simplified sulphur-iodine cycle flowsheet (McHugh *et al.*, 2005:3-7).

The heat needed for this process will most likely originate from high temperature gas-cooled nuclear reactors (HTGRs) such as a PBMR for example or the concentrated solar power. The high temperature at which the heat is required limits the choice of heat source. The possible nuclear reactors include heavy metal, molten salt or PBMR He-cooled reactors. Currently research into the use of helium (He) cooled reactors as heat source is investigated extensively and will most likely be the first heat source to be used.

The SI cycle is still in a research phase and technology needs yet to be proven. The current research is done at laboratory scale. The predicted thermal efficiency is 42 - 52% with an expected hydrogen production price of \$1.87/kg - \$2.01/kg (McHugh et al., 2005:3-9).

2.2.4 Hybrid Sulphur Cycle

The HyS is a thermochemical cycle that decomposes water into hydrogen and oxygen. The process consists of four sections namely: the decomposer, the sulphur dioxide (SO_2) and oxygen (O_2) separator, the electrolyzer and the concentrator. The net reaction of all the intermediate reactions is the dissociation of water to produce hydrogen. A simplified flowsheet of the HyS is represented in Figure 5.

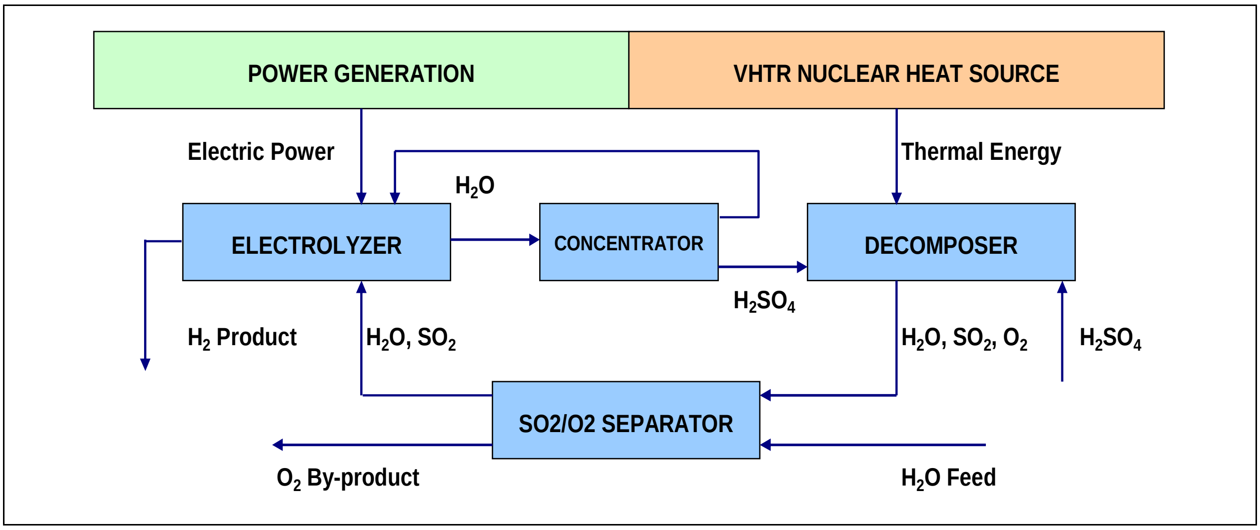

Figure 5: Simplified hybrid sulphur cycle flowsheet.

Concentrated sulphuric acid is fed into the decomposer at a specified pressure and temperature. The pressure is attained by a pumping action of the acid and the temperature is attained by the process heat from the nuclear plant's reactor coolant, in the form of hot helium. In the case of the PBMR, the process heat is in the form of hot helium gas. The sulphuric acid is vaporized and superheated causing it to spontaneously decompose. The sulphuric acid is decomposed into water and sulphur trioxide (SO_3) and when this mixture is further heated the sulphur trioxide is then decomposed into sulphur dioxide and oxygen in the presence of a catalyst. The two step decomposition reaction is described by the following:

$H_2SO_4 \leftrightarrow H_2O + SO_3$ (thermal decomposition >300℃) (8)

$SO_3 \leftrightarrow SO_2 + 1/2O_2$ (thermal decomposition, 870℃) (9)

The products leave the reactor in a gaseous form. It is then cooled to condense and separate the unreacted sulphuric acid from the sulphur dioxide and oxygen. The by-product, oxygen, is removed from the SO_2 and water (H_2O) mixture by means of compressing, a series of flash drums and a cryogenic cooling system. This occurs in the SO_2/O_2 separator section. The liquid mixture of SO_2 and H_2O are fed to the electrolyzer as the anolyte solution.

At the proton exchange membrane (PEM) electrolyzer, an electrode potential is used to decompose water into oxygen and hydrogen. At the anode, sulphur dioxide and water is oxidized and produce protons, electrons and sulphuric acid. The protons then diffuse through the membrane to the cathode. At the cathode, the protons recombine with electrons and are thus reduced to produce hydrogen gas. The reactions at the anode and cathode are given as follows:

Anode: $2H_2O + SO_2 \rightarrow H_2SO_4 + 2H^+ + 2e^-$ $E^o = -0.17V$

Cathode: $2H^+ + 2e^- \rightarrow H_2$ $E^o = 0.00V$

The overall electro-chemical reaction is:

$$2H_2O + SO_2 \leftrightarrow H_2SO_4 + H_2 \quad \text{(electrolysis, 100℃ – 120℃)} \qquad (10)$$

The dilute sulphuric acid produced by the electrolyzer is sent to the concentrator and the hydrogen gas is recovered as a product.

At the concentrator the dilute sulphuric acid is heated and flashed to remove the water. The water vapour is condensed and recycled to the electrolyzer and the concentrated sulphuric acid is sent to the decomposer.

The HyS process operating at 86 bar and a decomposition reactor temperature of 1143K, has a Higher Heating Value (HHV) thermal efficiency of 41.7% and a Lower Heating Value (LHV) thermal efficiency of 35.3%. A SO_3 conversion of 48.1% to SO_2 is achieved within the reactor at the above mentioned operating conditions (Gorensek & Summers, 2008:13).

2.3. Hydrogen from nuclear power sources

Most hydrogen is produced from natural gas and uses heat generated from fossil fuel power generation. Currently hydrogen production is expensive, which is counterproductive as far as stimulating the hydrogen economy is concerned. If the hydrogen economy is to succeed, more affordable feedstock and production methods are needed. Innovative technology that uses water as a feedstock and nuclear energy technology has to be further developed (Jeong *et al.*, 2005:1).

The use of nuclear hydrogen system integration will promote nuclear-based hydrogen production technologies. The major advantage of such an integrated system is low emissions of greenhouse gases (GHG). This makes it a favourable environmentally friendly technology. Other advantages include the sustainability of the technology and energy supply, as well as flexibility in the size of the production plant to meet the small and large production needs for specific markets (Yildiz *et al.*, 2005:1).

Nuclear technology for hydrogen production has to demonstrate commercial potential and technology readiness. Nuclear technology has been making progress in some of the advanced designs of nuclear plants. These nuclear plants can supply high temperature heat in the form of hot helium for hydrogen production. The potential designs are Gas Turbine Modular Helium Reactor (GTMHR) and HTGR (PBMR) (Jeong *et al.*, 2005:1).

2.4. Hydrogen Markets

The world consumes approximately 50 million tons of hydrogen per annum. Based on the current production methods this causes large volumes of greenhouse gas emissions and therefore large penalties to be paid in future. Penalties to be paid for CO_2 emissions are as high as $30/metric tonnes CO_2 (Gorensek *et al.*, 2009:89). Therefore the market for environmentally clean produced hydrogen is potentially significant (Forsberg, 2004:5).

Hydrogen has four major potential and existing markets. The first potential market is that of the transportation market. Liquid fuels such as gasoline, diesel and other oil-based fuels are the current leaders in the transportation market. These liquid fuels boast a high energy density, proven production technology and ease of use. Predictions, based on supply and demand of liquid fuels and reserves, indicate a rapid exhaustion of the liquid fuels. Consequently the oil companies have initialized an exploration for alternative transportation fuels and hydrogen has been identified as one of the options. Hydrogen has different options of use in this industry namely: liquid fuels (Coal-to-liquid, CTL), CO_2-free liquid fuels and direct hydrogen fuels (Yildiz *et al.*, 2005:87).

The second market of hydrogen is for industrial use. Two major industrial markets have been identified that can gain from the potential of hydrogen use. The current primary industry consumption of hydrogen is its use in fertilizer production. This industry consumes about half of the current hydrogen produced. The fertilizer industry is indicating a slow growth in the international sector but due to precision agriculture, predictions indicating a large growth of fertilizers is not expected (Yildiz *et al.*, 2005:96).

In the steel industry, the direct reduction of iron ore into iron and steel is achieved by means of syngas. Syngas is a mixture of hydrogen and carbon monoxide. The advantages of this method are lower capital costs and environmentally cleaner operations than blast furnace processes. Predictions indicated that the use of syngas will continue to rise at the cost of conventional production process (Yildiz *et al.*, 2005:96-97). Unlike electricity, hydrogen can be stored and used on demand.

The electricity sector is another potential market user of hydrogen. Electricity demand and prices varies as a function of time. The high demand periods have expensive tariffs. During these peak periods some form of extra electricity generation is necessary. Some utilities use pumped hydro storage facilities to meet the extra demand. The potential for hydrogen is to supply the utilities with peak electricity production. A nuclear hydrogen integrated system will be used to produce hydrogen during low-cost power periods and store it in underground facilities. During peak power periods, large banks of fuel cells will convert the stored hydrogen to electricity (Yildiz *et al.*, 2005:82,98).

The fourth potential hydrogen market is for commercial applications in buildings. Once the most cost effective technologies for production of hydrogen have been developed and proven, hydrogen can be use to generate electricity, building heating and cooling and for heating of water for individual use. The bulk of hydrogen usage will require the development of small-scale fuel cells but the potential market is substantial (Yildiz *et al.*, 2005:85,100).

A factor to take into consideration when discussing hydrogen economy is the storage of hydrogen and its requirements. Hydrogen storage is a relevant goal in the development of the hydrogen economy. Often it is found that literature compare the gate hydrogen price to the gallon of gasoline equivalent (gge) price. This however is not correct as in most cases hydrogen product requires some compressing or liquefaction and storage in order to deliver it at usable pump pressures (350-700bar). This increases the cost of the hydrogen and should only be compared to gge at this pump pressure conditions. Hydrogen can be stored in a compressed or liquefied form, called physical storage, or in hydride form, called chemical storage. Each comes with its difficulties.

The challenge of hydrogen storage lies in its characteristic that it has the highest energy content per unit of weight of any known element and also the lightest element. Thus hydrogen has a low volume energy density, meaning that a given volume of hydrogen contains a small amount of energy. As a result large storage volumes will be required to store the amount of energy required to drive the hydrogen economy. Other challenges for the transportation sector is to balance the vehicular constraints of weight, volume, efficiency, safety, and the cost of on-board hydrogen storage systems with the need for a conventional driving range (>480 km).

2.5. *Previous studies undertaken*

2.5.1 Technical Evaluation

A study done on the “Hybrid sulphur flowsheets using PEM electrolysis and a bayonet decomposition reactor” by Gorensek and Summers (2008:4097) determined the proposed hybrid sulphur cycle flowsheet and the operating conditions for hydrogen generation. This technical evaluation lead to a conceptual design for the hybrid sulphur process. The production of hydrogen involves using a high temperature nuclear heat source to split water into hydrogen and oxygen.

The study made use of the Aspen Plus^{TM} software package with the model OLI Mixed Solvent Electrolytes to develop the flowsheet. The main focus points within the cycle were the bayonet decomposition reactor and the proton exchange membrane-based SO_2-depolarized electrolyzer technology. The other sections namely the separation section and the concentration section, made use of proven and existing technology. The electrolyzer product is concentrated from 50 wt% to 75 wt% by means of a vacuum distillation. The separation of SO_2 and O_2 is performed by means of a series of flash drums using a vapour/liquid split and an absorber column.

The bayonet reactor is operated at 86 bar and 1,143K (870℃). The overall conversion of H_2SO_4 to SO_2 achieved in the reactor is 48%. The electrolyzer is operated at 100℃ and 21 bar. The electrolyzer is t reated as a black box since the detail model of the SDE has not been developed. The conversion of SO_2 in the electrolyzer totals to 40% and a net flux of H_2O from the cathode to the anode occur at a rate of 1 kmol H_2O per kmol of SO_2 reacted.

In the proposed HyS an energy consumption of 120.9 kJ electric power, 340.3 kJ high temperature heat, 75.5 kJ low-temperature heat and 1.31 kJ low pressure steam for every mol H_2 produced were obtained. A Lower Heating Value (LHV) thermal efficiency of 35.3% and a Higher Heating Value (HHV) thermal efficiency of 41.7% is achieved with an electric power conversion efficiency of 45%.

The study gave insight into the simulation requirements for achieving an accurate model. The results obtained in the study from the various potential models that can be used for the simulation will be applicable to the study at hand.

Another study done on the "Optimization of the hybrid sulphur cycle for hydrogen generation" by Jeong *et al.* (2005:ii) determined the optimal operating conditions for hydrogen generation. This technical evaluation of the HyS explored ways to optimize the energy efficiency of the process. This was achieved by varying the electrolyzer and decomposer acid concentration, the pressure and temperature of the decomposer and internal heat recuperation.

The study determined that for high acid concentrations, the energy demand of the decomposer and concentrator diminishes but power demand increases for the electrolyzer. For a low acid concentration the electrolyzer power demand will be low but the mass flow through the system will increase due to the high volume of water associated with low acid concentration. This will also increase the thermal demand per unit hydrogen production of the decomposer due to the higher heat capacity needed to heat up water compared to heating sulphuric acid.

The temperature of the system is another factor that influences the cycle thermal efficiency. The study determined that for a high temperature the decomposition rate of sulphuric acid in the decomposer increases, implying that a lower recycle rate is achieved. This in effect will also increase the possible thermal efficiency of the cycle.

Pressure is yet another operational condition that was under investigation. For a high decomposer temperature, without considering the pressure, a high decomposition rate can be achieved. At a given temperature a high decomposer pressure yields a lower SO_3 production. A lower SO_3 yield causes a lower SO_2 yield which causes a lower hydrogen production rate.

The lower SO_3 yield due to high decomposer pressure causes a lower compressor power in the SO_2/O_2 section. The lower compressor power is due to a lower mass flow of SO_3 and this allows for less energy needed to lower the temperature of the mixture.

On the other hand, low decomposition pressure allows for high decomposition of sulphuric acid, causing a high yield of SO_3 and SO_2, in turn causing a high power demand by the compressor.

The study showed a research methodology that can be successfully applied for the technical evaluation of the mini-dissertation. The study also gave insight into the operation of the process and the operating conditions of the HyS.

2.5.2 Economic Evaluation

A study by Gorensek *et al.* (2009:1) on the “Hybrid Sulphur Process Reference Design and Cost Analysis” performed a cost estimation of the HyS process by using process heat supplied by a PBMR.

The proposed nuclear reactor is a high temperature reactor with helium gas as coolant. The coolant from the reactor is used as process heat for the HyS cycle. The coolant outlet temperature is approximately 900ºC. The proposed hybrid sulphur cycle operates at a temperature of 870ºC and at 86 bar for the SO_3 decomposer. The HyS is based on a production rate of 160.1 MT/day hydrogen with a process thermal efficiency of 36.7% based on the HHV of the hydrogen product.

The study estimated the total direct depreciable cost for a HyS processing plant that produces a total of 160.1 MT/day H_2 to be $460 million. The study further estimated the total direct depreciable cost for a nuclear heat supply system (NHSS) to be $450 million, the power generation system (PGS) costs $57million and the balance of plant (BOP) costs $147 million. The CAPEX of an integrated PBMR HyS water splitting system, including the indirect costs, contingency and land totals to $1,240 million. The configuration of the integrated PBMR HyS and the equipment involved to arrive at the estimation, is illustrated by Figure 6 below.

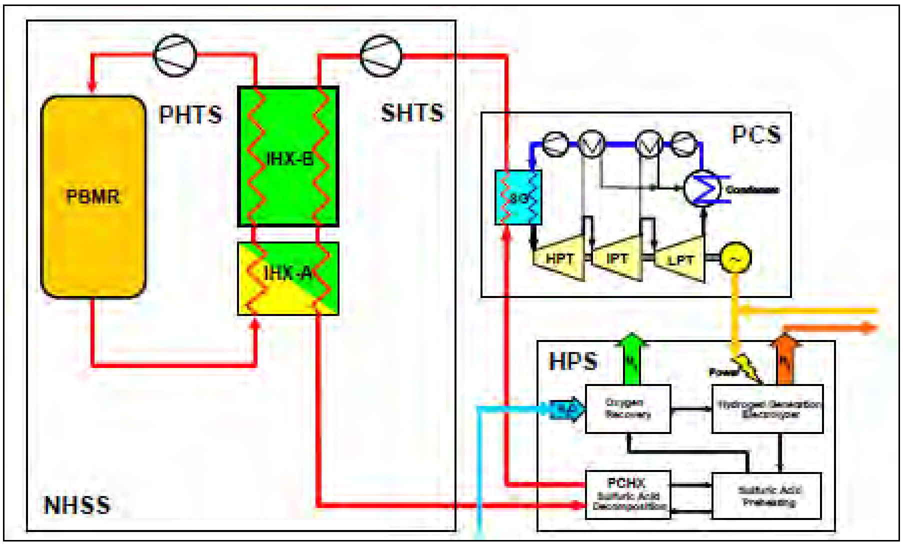

Figure 6: PBMR HyS Plant Schematic Configuration (Gorensek *et al.*, 2009).

The costs for the acid decomposer equipment were based on a recuperative reactor design. The cost estimation was given by Westinghouse Electric and includes the catalyst costs. The remaining equipment cost estimation for the HyS hydrogen processing system (HPS) was calculated by Gorensek *et al.* (2009:73-74) by means of the program Factored Automated Cost Estimating System (FACES). This program is based on Shaw's practical experience on cost estimation of equipment and projects.

The direct depreciable costs cited in this study include the following:

- Uninstalled plant component costs – equipment costs.
- Installation costs:
  - Direct labour.
  - Indirect labour.
  - Expenses of installation.
  - Engineering.
  - Management of installation.
  - Field bulk material.
  - Spares.
  - Freight.
  - Other cost elements.

The indirect costs cited by the study include the following:

- Engineering services.

- Indirect construction costs.
- Facilities.
- Tools.
- Insurance.
- Building permits.
- Taxes.
- Field Office:
    - Management.
    - Startup and testing.
    - Quality control.
- Home Office:
    - Project development and management.
    - Nuclear licensing and permitting.
    - Quality assurance and configuration control.
- Owners' Costs:
    - Management.
    - Training.
    - Startup expenses.
    - Consumables.
    - Initial reactor cores.
    - Initial fluid can chemical inventory.
    - Spares.

The conclusion of the study indicated that for a HyS with a plant life of 40 years, the plant will have an Internal Rate of Return (IRR) of 10% for a 7.4kg/s hydrogen production plant. The facility consists of four 160.1 MT/day HPS modules with its 4-unit NHSS and other requirements. The hydrogen cost of production delivered by this study for the above-mentioned PBMR HyS water splitting plant is presented in Table 1 below.

Table 1: Hydrogen Price Components Detail in $/kg Hydrogen (Gorensek *et al.*, 2009).

PBMR HyS Water Splitting Plant	NHSS	HPS	PGS	BOP	Other	Total	%
	$/kg	$/kg	$/kg	$/kg	$/kg	$/kg	
Capital Charge	1.55	1.57	0.19	0.5	0.22	4.03	65
Fixed O&M: Labor, Taxes, Insurance, Annual Licensing, Permits and Fees, Material Costs for Maintenance and Repairs, Nuclear Decommissioning Funding, Helium Make-up	0.1	0.08	0.01	0.03	0.47	0.69	11
Variable O&M Nuclear Fuel, Process Catalyst and Chemical Consumption and Waste Disposal	0.41	0.15	-	0.01	-	0.57	9
Utilities and Feed Electric Power and Process Water	0.34	1.49	-0.62	0.02	-	1.23	20
Byproduct Credit (O_2)	-	-0.32	-	-	-	-0.32	-5
Total Hydrogen Cost	2.4	2.97	-0.42	0.56	0.69	6.20	100

The cost for producing hydrogen totals to $6.20/kg hydrogen. The costs for only hydrogen production excluding the nuclear heat and capital for a NHSS, PGS and BOP equals to $3/kg hydrogen. Of this the capital charge contributes the highest amounting to 52.8%. The utilities, feed and electric power contributes 50.2% followed by the variable costs with 5% and the fixed costs with 2.7%. The by-product oxygen contributes to 10.7% deduction in the hydrogen production price (credit of $0.32/kg assumed).

Another study by Summers *et al.* (2005:1) "The hybrid sulfur cycle for nuclear hydrogen production" investigated the two leading processes required for hydrogen production. The two processes are the hybrid sulphur cycle (HyS) and the sulphur iodine cycle (SI). The study prepared an estimate for the capital costs and hydrogen production costs for an Nth-of-a-kind nuclear hydrogen production plant for the HyS cycle. The plant design consists of four nuclear reactors to supply process heat and electricity together with the HyS process. The thermal efficiency of the cycle was estimated at 48% and the plant was sized for 580 metric tonnes per day. The study determined a value of $516 million for the total installed capital cost of the HyS cycle and a $1.2 billion for the total installed capital cost for the nuclear reactor system.

The operational costs of the cycle were also estimated by the study. A hydrogen production cost of $2.97 per kilogram, excluding NHSS, PGS, BOP and other costs, was determined. This value includes all nuclear fuel costs, capital recovery charges, operating costs and maintenance of the cycle costs.

These studies showed the research methodology for an economic evaluation of the hybrid sulphur cycle.

CHAPTER 3

HYBRID SULPHUR CYCLE

3. Proposed Hybrid Sulphur Cycle (HyS)

Chapter 2 gave a literature review on the various methods that could be used to produce hydrogen. The methods can be categorized into two groups namely fossil fuel sources and nuclear or alternative energy sources. The chapter also investigated the previous work done on cost analysis and economic evaluation of the HyS proposed by Savannah River National Research Laboratories (SRNL). The chapter also looked at previous technical evaluation studies done on the HyS. The studies gave insight into the working of the process and the operating conditions of the HyS and also showed a research methodology that could be applied for the technical evaluation of this mini-dissertation. The nuclear power sources for hydrogen production were also discussed in the chapter.

Chapter 3 will give a detailed description of the hybrid sulphur cycle. Process conditions and cycle efficiency will be discussed in the chapter as well as the assumptions made as basis for the development of the proposed process flow sheet.

The hybrid sulphur cycle can be described by following two reactions:

$$H_2SO_4 \leftrightarrow H_2O + SO_3 \leftrightarrow SO_2 + 1/2O_2 + H_2O \quad (11)$$

$$2H_2O + SO_2 \leftrightarrow H_2SO_4 + H_2 \quad (12)$$

The HyS cycle consists mainly of four process steps, namely the decomposer, the separator, the electrolyzer and the concentrator. The first step is the decomposition of sulphuric acid into sulphur trioxide and water. The sulphur trioxide is then further decomposed into sulphur dioxide and oxygen. The process stream is cooled and the separation of sulphuric acid (liquid) from sulphur dioxide (gas) and oxygen (gas) is done in separation tanks. The sulphur dioxide and oxygen are then separated from each other by means of cryogenic cooling. The oxygen could be sold as a by-product. The sulphur dioxide, water and trace amounts of oxygen are routed to the electrolyzer, where the third process step takes place. The electrolyzer uses water and sulphur dioxide to generate hydrogen. Sulphur dioxide is fed to the anode where it is electrochemically oxidized to produce sulphuric acid, protons and electrons. The protons generated at the anode are then conducted across the membrane to the cathode. At the cathode the protons recombine with the electrons to form hydrogen.

The sulphuric acid, produced at the anode, is pumped to the fourth process, the concentrator, while the hydrogen, produced at the cathode is routed to a purification process and recovered as pure hydrogen. The dilute sulphuric acid is concentrated and eventually recycled to the decomposer reactor. The concentrator pressurizes, heats and flashes the dilute sulphuric acid produced by the electrolyzer to produce a concentrated sulphuric acid, 80-90 mol% H_2SO_4, needed for the decomposer section.

3.1 Decomposer Section

The recycled sulphuric acid from the concentration section is routed to the decomposer section once the required sulphuric acid concentration is achieved. The feed (101) to the decomposer section, presented by Figure 7, is a 70% - 80% mol concentration sulphuric acid at 1 bar and 166℃ in a liquid form. The feed containing 1,350 mol/s H_2SO_4 is routed to pumps (P-101, P-102) where the stream is pressurized to the operating pressure of the first reactor (RX-101). The pressurized stream is preheated by heaters (HX-101, HX-102), followed by the vaporizer (HX-103) to achieve a gaseous stream. HX-103 makes use of the nuclear heat source to perform its heating function. The vaporized stream is further heated by a counter-flow heat exchanger before being routed to a sulphuric acid decomposer reactor. During the vaporization of the stream, the decomposition of the concentrated sulphuric acid commences and continues until the stream reaches the sulphur trioxide reactor. The decomposition reaction is a reversible reaction and is simulated as such. Equilibrium conversions for reaction (13) are applied within the simulation. The reactors in the decomposition section are modelled as counter-flow heat exchanger reactors with the feed stream heating performed by an incoming nuclear heat source, being hot helium. The nuclear heat source allows the reactors to achieve the required temperature and also assists to heat other reaction streams to the desired operating temperature. The sulphuric acid decomposition reaction is a reversible endothermic gas phase reaction where sulphuric acid is decomposed to sulphur trioxide and water. The reaction is given as follows:

$$H_2SO_4\,(g) \leftrightarrow SO_3\,(g) + H_2O\,(g) \qquad \Delta H_r = +97.54\ \text{kJ/kmol} \qquad (13)$$

The product stream from the sulphuric acid reactor (RX-101) contains sulphur trioxide, water and unreacted sulphuric acid. The stream is fed into a second counter-flow heat exchanger before being routed to the second reactor (RX-102), the sulphur trioxide reactor. The unreacted sulphuric acid continues to decompose within the heat-exchanger before entering RX-102. Once the stream enters the second reactor, the sulphur trioxide mixture starts to decompose into sulphur dioxide and oxygen. This reaction is an endothermic gas phase reaction that takes place in the presence of a catalyst.

$$SO_3 \rightarrow SO_2 + \frac{1}{2} O_2 \qquad \Delta H_r = +98.92 \text{ kJ/kmol} \qquad (14)$$

The product stream from the second reactor consists of unreacted sulphuric acid, unreacted sulphur trioxide, sulphur dioxide, oxygen and water. The product stream is then routed to the counter-flow heat exchangers (HX-101,HX-102) for heating the incoming feed stream and thereby achieving efficient use of the available heat added to the cycle. During the flow through the counter-flow heat exchangers the hot product stream transfers heat to the feed stream. During the cooling phase the unreacted sulphur trioxide to react with water to produce sulphuric acid. Once the stream has moved through the heat exchangers, the stream is routed to the separation section where the dilute sulphuric acid is removed and routed to the concentration section, the oxygen is separated and recovered as a by-product and the sulphur dioxide and water mixture is routed to the electrolyzer section.

Due to the endothermic nature of the reactions taking place within the reactors, a heat source capable of heating the stream to temperatures as high as 870℃ is required. The proposed heat source will be hot helium from a Very High Temperature Reactor (VHTR) such as a PBMR. The helium is the coolant used in the PBMR and is fed to the HyS system at a rate of 160kg/s at 900℃. The helium could provide 500 MWt of thermal energy to the HyS plant. The reactors will also make use of the helium to heat the incoming stream to the required operating temperatures.

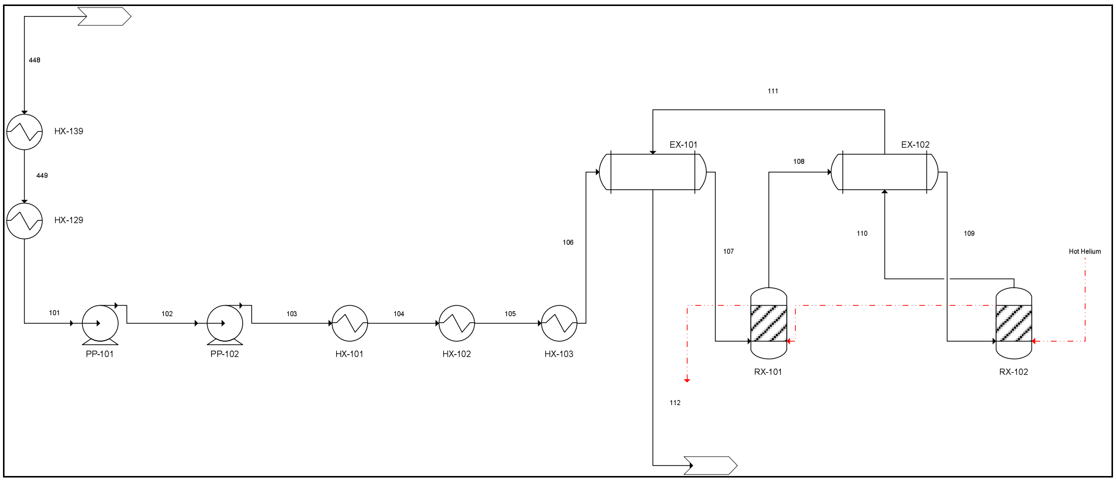

Figure 7: HyS Decomposer Section.

3.1.1 Decomposer section efficiency parameters

The overall efficiency of the HyS depends mainly on the efficiency of the sulphuric acid decomposition and the sulphur trioxide decomposition reactor systems. The reactions and the kinetics involved are of a high endothermic nature. The equilibrium conversion of sulphuric acid to sulphur trioxide at various operating pressures as a function of temperature is given in Figure 8.

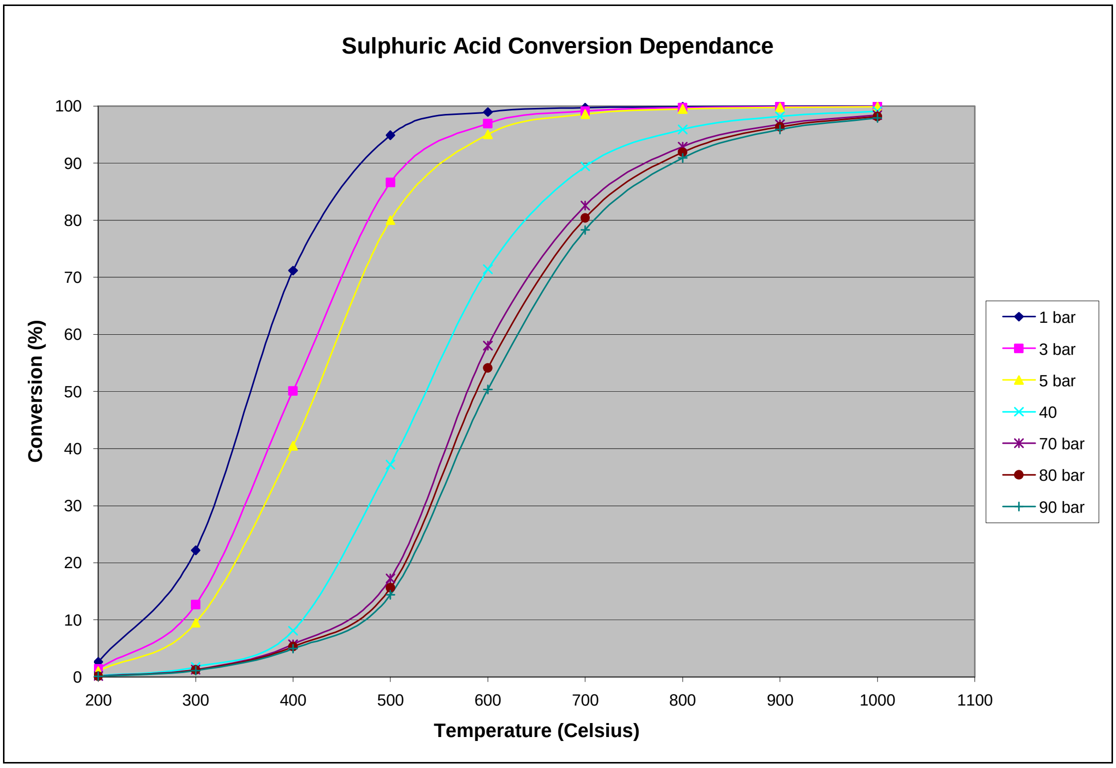

Figure 8: Equilibrium conversion of sulphuric acid decomposition.

The equilibrium conversion of sulphur trioxide to sulphur dioxide at various operating pressures as a function of temperature is given in Figure 9.

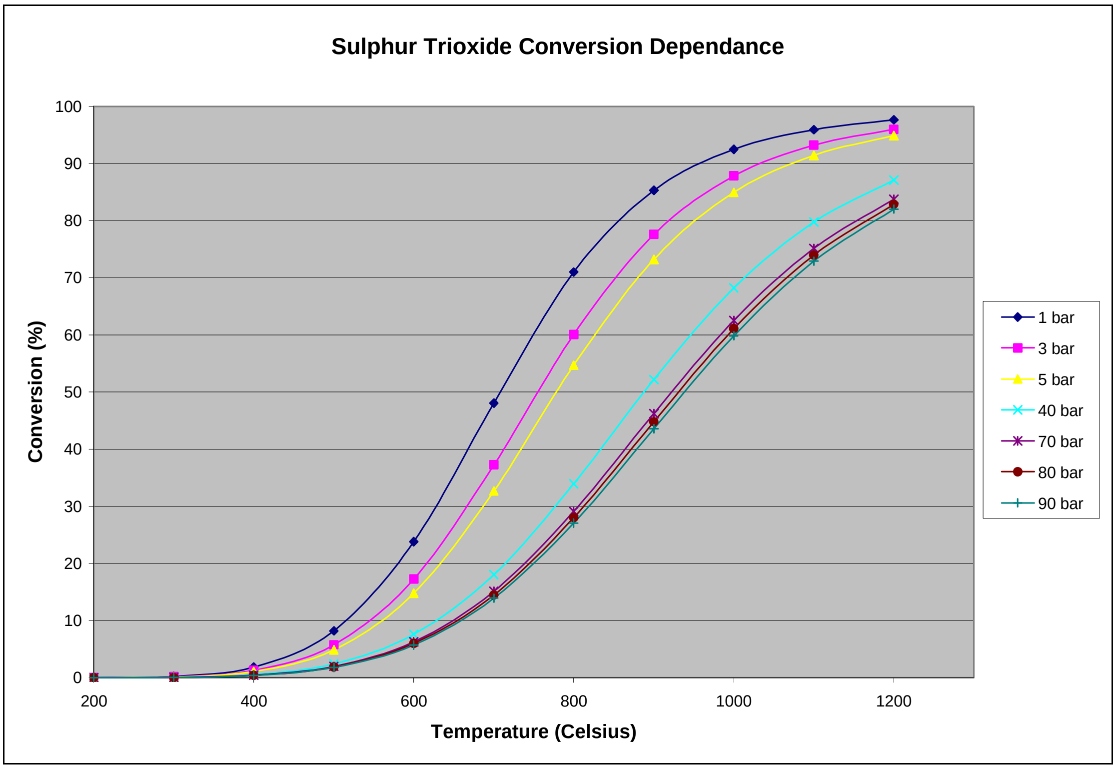

Figure 9: Equilibrium conversion of sulphur trioxide decomposition.

The equilibrium conversion figures clearly indicate that the decomposition of sulphuric acid and sulphur trioxide are dependent on the operating temperature and operating pressure of the reactors. Figure 8 indicates that to achieve a high conversion of sulphuric acid at a high pressure, a high operating temperature is required. For example, at a temperature of 550℃ a low operating pressure (1-5 bar) is required in order to achieve a conversion of 90%. In the case of operating at 90 bar, a temperature higher than 700℃ is required to achieve a conversion of 90%. A similar dependency on the conversion efficiency by the operating temperature and pressure can be observed in Figure 9 for the decomposition of SO_3 to SO_2.

The operating pressure of the reactors also have other effects on the process efficiency. The effect will be observed in the separation section. In order to separate O_2 and SO_2, low temperatures and high pressures are required. Therefore operating the reactors at low pressures will require higher power conditions for the compressor system within the separation section. This will have a negative effect on the cycle thermal efficiency.

The feed concentration of sulphuric acid also influences the cycle efficiency. Previous studies have shown that a concentration of 80 mol% will allow for higher thermal efficiencies to be achieved. The lowest heating target of 330kJ/kmol SO_2 were obtained for feed concentrations of 80% at all pressures (Gorensek *et al.*, 2009:25).

3.1.2 Assumptions within the Decomposer section:

The following assumptions have been made:

- No heat loss from the heat-exchangers and the reactors to the environment was assumed. This assumption allows the study to determine the maximum theoretical thermal efficiency.
- Helium is fed from its source to the HyS reactor section at 160kg/s at 900℃. The helium will deliver 500 MWt of thermal energy (A 500 MWt HTGR).

3.2 Separation Section

The reactor effluent can easily be separated into the unreacted H_2SO_4 and the SO_2/O_2 mixture. This is achieved by performing a vapour-liquid split. The reactor effluent is firstly cooled to 120℃ in heat-exchang ers HX-104, HX-105 and HX-106, illustrated in Figure 10. This allows the unreacted sulphuric acid and water to condense as well as the unreacted sulphur trioxide to react with water producing dilute sulphuric acid while the SO_2/O_2 mixture remains in vapour form. The stream 215 is then routed to flash drum FL-101 which allows the liquid and vapour phase to separate. The dilute sulphuric acid is then routed to the concentration section while the SO_2/O_2 mixture is routed to compressor CO-101 where the stream is compressed to 21 bar. This compression is done to achieve the same pressure conditions as that of the electrolyzer section. This compression action causes the stream to be heated. In order to achieve separation of sulphur dioxide from oxygen, a lower temperature is needed. Heat exchangers HX-107, HX-108 and HX-109 cool the stream to 40℃. This causes the sulphur dioxide to condense while the oxygen remains in vapour form. The flash drum FL-102 allows the vapour phase to separate from the residual liquids. Stream 217 is routed to the anolyte tank (TK-101). Stream 216 is fed to a cryogenic cooling system that cools the stream to -23℃. At these temperatures all impurities are liquefied while oxygen remains in a gaseous form. Flash drum FL-103 allows the vapour phase to split from the residual liquids. The liquid stream is routed to the anolyte tank. The oxygen rich stream is fed to the O_2 dryer (DR-101) where the remaining SO_2 and H_2O are removed and routed to the anolyte tank. Eight tons of oxygen are produced for each ton of hydrogen. The oxygen by-product is recovered and could be sold.

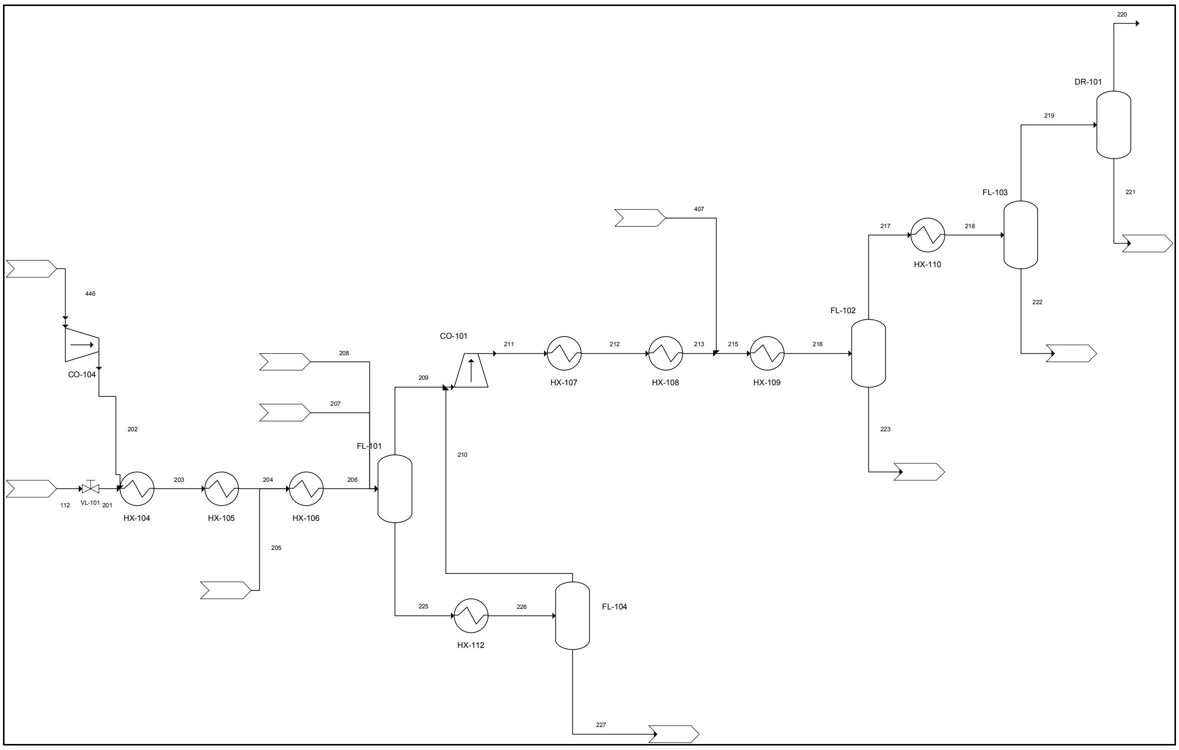

Figure 10: HyS Separation Section.

3.2.1 Separation Section Efficiency Parameters

The efficiency of the separation cycle largely dependents on the working conditions of the compressor CO-101. CO-101 is used to pressurize streams 208 and 209 to the operating pressure of the electrolyzer. The electrical power needed for the compressor is directly related to the pressure difference between the inlet and outlet of the compressor. It can be concluded that, for a higher operating pressure in the reactors, a lower power requirement will be needed for the compressor with a corresponding lower conversion of sulphuric acid and sulphur trioxide. This level of conversion will be reflected on the amount of electricity that will have to be imported or exported by the process.

3.3 Electrolyzer Section

The effluent from the separation section is fed to the anolyte tank, TK-101, which contains a mixture of sulphur dioxide, water and trace amounts of oxygen. The flowsheet is illustrated by Figure 11. Streams 301 and 302 are the feed streams to the electrolyzer anode. The electrochemical reaction that takes place is the SO_2-depolarized electrolysis of water. The half-cell reactions are:

Anode: $SO_2\ (aq) + 2H_2O(aq) \rightarrow H_2SO_4\ (aq) + 2H^+ + 2e^-$

Cathode: $2H^+ + 2e^- \rightarrow H_2$

Net Reaction: $SO_2\ (aq) + 2H_2O \rightarrow H_2SO_4\ (aq) + H_2\ (g)$

At the anode the SO2 feed reacts with water to produce sulphur trioxide and protons. Sulphur trioxide produced in the anode reacts with water to produce an aqueous sulphuric acid solution. The protons are positively charged and are therefore attracted to the negative cathode charge. The protons are conducted across the proton exchange membrane (PEM), also known as the electrolyte separator. The protons react with the electrons at the cathode to produce the hydrogen product. The SO_2-depolarizer electrolyzer (SDE) membrane must be kept moisturized to allow protons to be conducted across. The electrolyzer therefore also experiences a net flux of water from the anode to the cathode. A net flux of 1kmol H_2O/kmol SO_2 reacted occurs. This flux occurs due to a difference in water activity across the PEM.

A mixture of H_2 and H_2O exits the cathode at 100℃ and 20 bar. The hydrog en rich stream is cooled by HX-112 to 75℃ allowing the wat er within the stream to condense and be removed by the flash drum FL-105. The light key component, hydrogen, is removed by the flash drum and fed to the H_2 Dryer DR-102. The H_2 Dryer cools the stream to 40℃ with cooling water causing the remai ning water to condense and deliver a high purity hydrogen product. The water removed is recycled back to the electrolyzer.

The flowsheet for the electrolyzer section is illustrated in Figure 11.

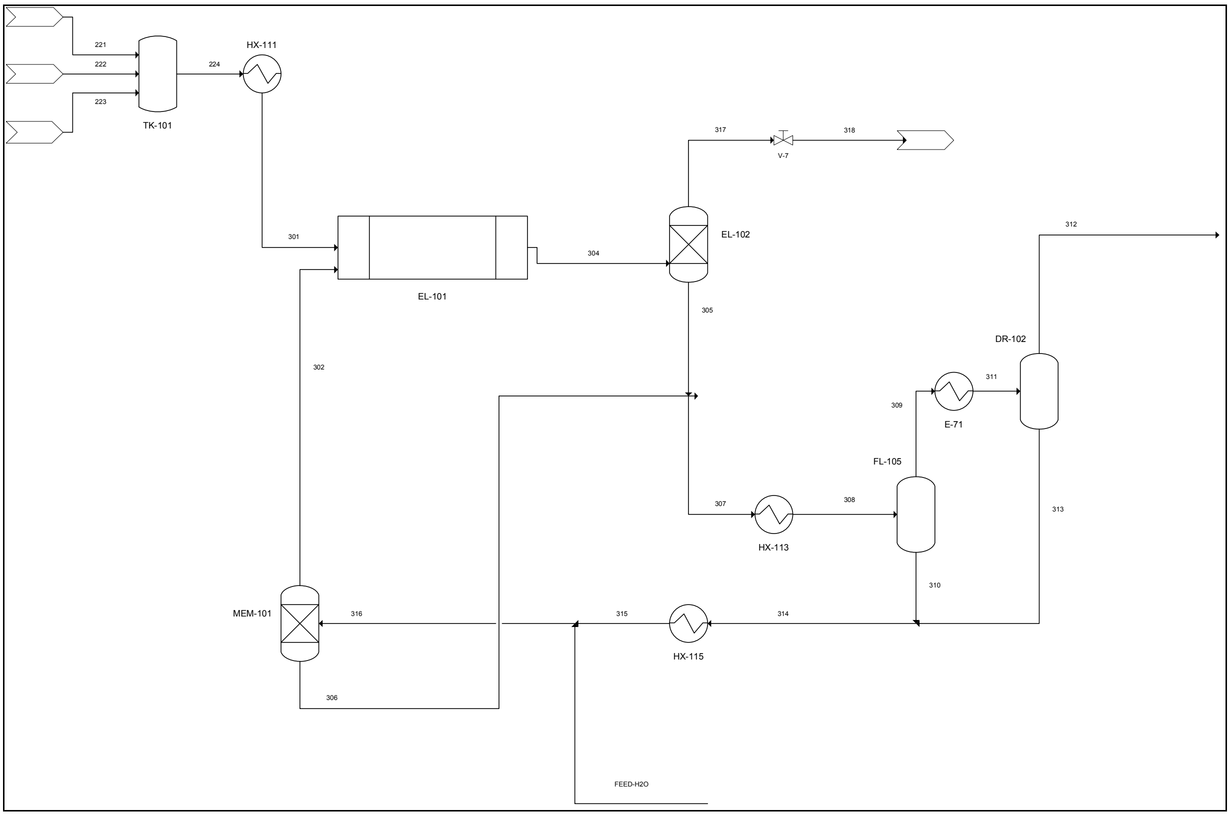

Figure 11: HyS Electrolyzer Section.

The net reaction of the electrolyzer is the production of sulphuric acid at the anode and hydrogen at the cathode. The basic operation of the electrolyzer is illustrated in Figure 12.

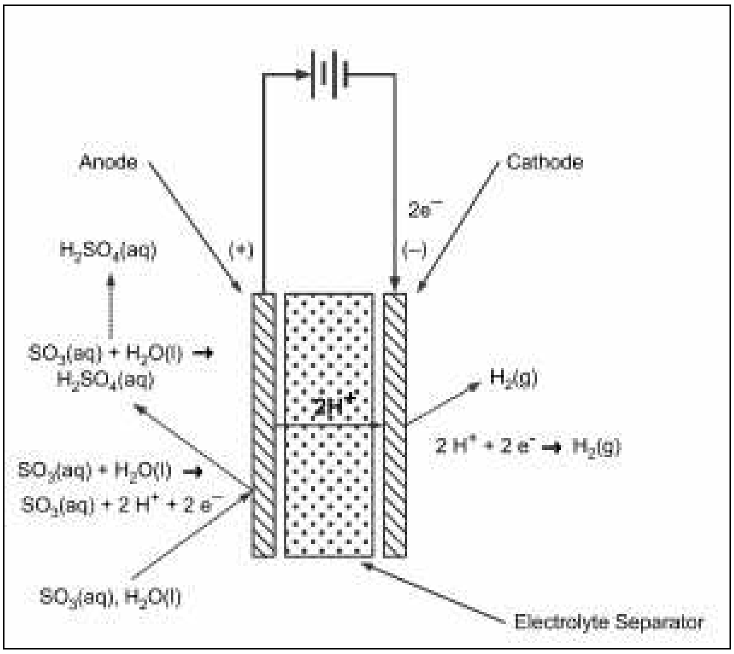

Figure 12: SO_2-Depolarized Electrolysis (Gorensek and Summers, 2008).

The electrolyzers' power requirements are highly dependent on the total voltage of the cell. The theoretical voltage required for hydrogen production in the absence of sulphur dioxide is 1.23V and only 0.17V in the presence of sulphur dioxide at the anode.

The electrolyzer's theoretical standard cell potential of -0.158V at 25℃ in water is required for the HyS cycle. A reversible potential of -0.243V is achieved in the presence of SO_2. When this is compared to water electrolysis reversible cell potential of -1.229V it can be concluded that SDE will require less electricity per mol hydrogen produced.

For the HyS, SRNL predicts that the cell potentials of -0.6V could be obtained at practical current densities of 500mA/cm^2 with the electrolyzer operating at higher temperature (>100℃) and higher pressures (>10 bar) . This low cell voltage will make the HyS more attractive than the opposing water electrolysis process.

3.3.1 Electrolyzer Section Efficiency Parameters:

The factors that influence the efficiency of the electrolyzer are the operating temperature, pressure and the concentration of sulphuric acid. It can be observed that the quantity of sulphuric acid produced within the electrolyzer is directly related to the electrical requirements of the electrolyzer. A higher amount of sulphuric acid produced is due to a higher volume of SO_2 reacted, which produces hydrogen. A higher volume of hydrogen produced results in a higher number of electrons that combine with the protons which directly relates to the amount of electricity being used.

Other studies by Ni *et al.* (2008:2751) also indicate that a higher operating pressure causes a lower cell potential over the electrolyzer.

3.3.2 Assumptions within the electrolyzer section:

The following assumptions have been made:

- The SDE has been modelled as a "black box".
- A net flux of H_2O from the cathode to the anode is due to a difference in water activity across the PEM. Assume a flux of 1kmol H_2O/kmol SO_2 reacted.
- Assumed SO_2 conversion of 40% at 100℃ and 20 bar.

- All the hydrogen produced exits the electrolyzer at the cathode.
- The remaining effluent exits the electrolyzer at the anode.
- Assume no heat loss to the environment.
- The electrolyzer is operated at 20 bar.
- The temperature of the SDE is maintained at 100℃ by controlling the temperature of the anolyte feed.

3.4 Concentration Section

The concentration section, illustrated by Figure 13, is fed by two streams: the anolyte effluent from the electrolyzer and the heavy key component from flash drum FL-101 which contains dilute sulphuric acid. There are various methods available to concentrate sulphuric acid. Sulphuric acid concentration can be achieved by either maintaining the temperature at 100℃ and releasing the pressure to 0.05 bar or by maintaining the pressure at 20 bar and increasing the temperature to >300℃. These actions cause water to boil allowing the vapour phase to be separated by means of a series of flash drums. The concentration of sulphuric acid is an energy intensive process. This section will have a significant influence on the energy requirement of the HyS.

The anolyte effluent is heated to 90℃ vaporizing SO_2. Flash drum FL-106 split the heavy key components, H_2SO_4 and H_2O, from the light key component, SO_2. The light key components are cooled by heat-exchanger HX-117 before being fed to flash drum FL-107. The vapour phase from FL-111 is also fed to FL-107. FL-117 vapour phase contains concentrated SO_2 and the liquid phase contains impurities to the SO_2 stream. The vapour phase is routed to compressor CO-102 and heater HX-118 to produce a concentrated SO_2 stream at 20 bar and 100℃. Flash drum FL-108 is the last component used to remove some water from the SO_2 stream. The vapour phase of FL-108 contains a concentrated SO_2 stream that is routed to the SO_2/O_2 separation section.

The liquid phase from flash drum FL-101 containing dilute sulphuric acid is heated in order to boil the water component and remaining SO_2. Flash drum FL-104 separates the boiled off water and SO_2 in a vapour phase from the liquid phase sulphuric acid. The vapour phase is routed to compressor CO-101 to recover the SO_2 remaining in the stream. The liquid phase is routed to a series of flash drums, FL-111 and FL-112, where the pressure is dropped to 1 bar and 0.3 bar respectively. This action boils off the water component within the stream and is removed by means of the flash drums. The vapour phase from FL-111 is cooled to 70℃ by heat-exchangers HX-121,HX-122 and HX-123 before being fed to FL-107. The vapour phase from FL-112 is also cooled by heat-exchangers HX-124 and HX-125 to 40℃ before being fed to FL-110. The liquid phase sulphuric acid is routed to flash drum FL-113 for further concentration.

The liquid phase of flash drum FL-113 is pressurized by pump PP-104 to 1 bar and heated by heater HX-127 to 306℃. This action causes the boiling of the water component within the stream. The liquid phase of flash drums FL-114 and FL-115 contains a concentrated sulphuric acid component. The 80 mol% sulphuric acid is heated by HX-129 and HX-130 and pressurized by pumps PP-101 and PP-102 to the operating conditions of the reactor RX-101. The concentrated sulphuric acid stream is routed to the reactor section.

The basic operation of the concentration section is illustrated in Figure 13.

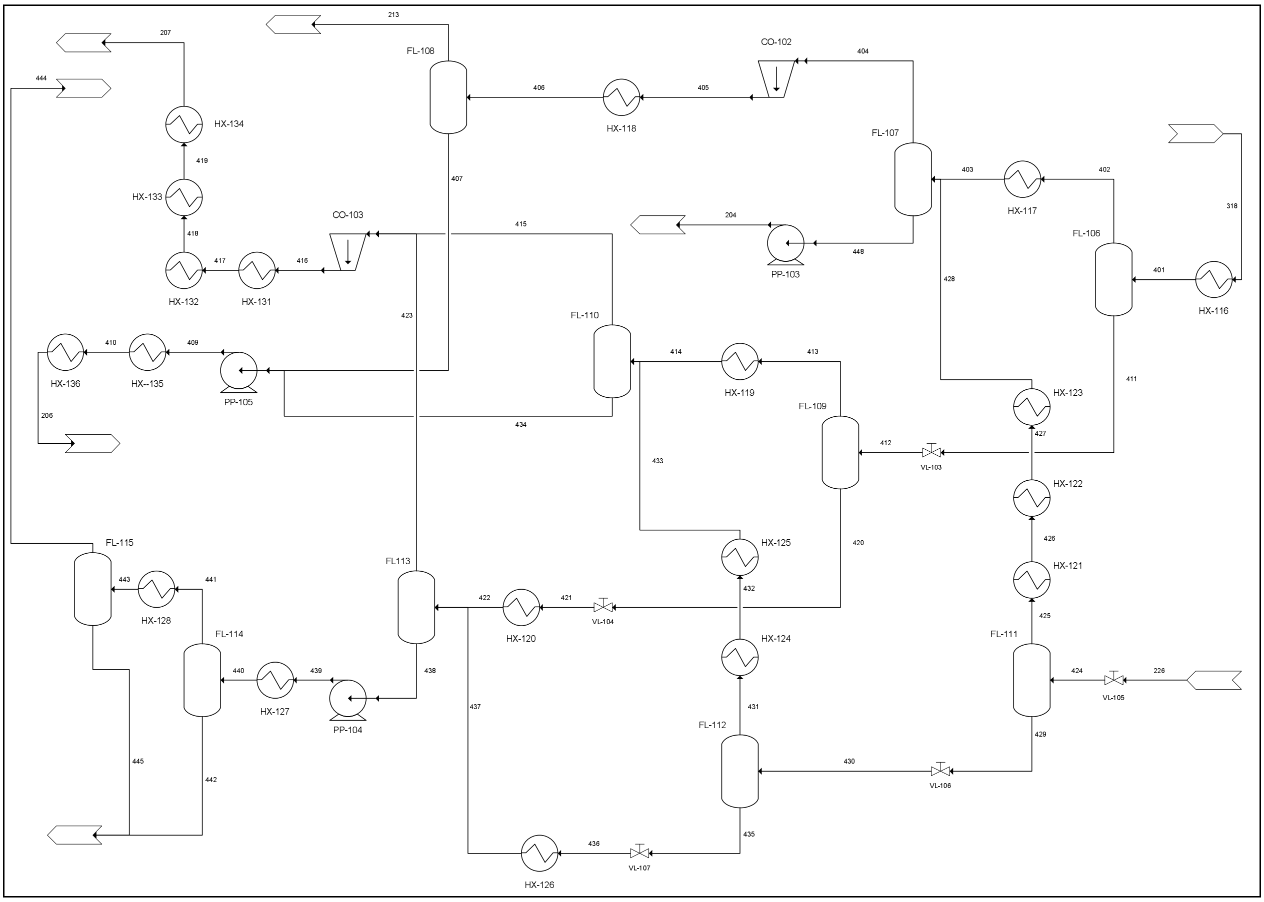

Figure 13: HyS Concentration Section.

3.4.1 Concentration Section Efficiency Parameters:

The concentration section has a significant influence on the efficiency of the cycle. Due to the heating, cooling, pressurization and compression of the streams, the power requirements of the cycle depends heavily on the operating conditions and feed concentrations of the reactors and the electrolyzer. For a high concentration of sulphuric acid feed to the reactors, a high thermal efficiency can be obtained due to the smaller amount of water that needs to be heated together with the sulphuric acid. This will, however, increase the energy requirements as higher temperature conditions are needed to obtain higher levels of sulphuric acid concentrations.

Another factor that influences the cycle efficiency is the operating pressure of the reactors and the electrolyzer. The concentration section will increase its power requirements in case of a high operating pressure within the reactor and electrolyzer. The lower the operating pressure the lower the compressor work requirements and the lower the heating load.

3.5 Analysis

An Aspen Plus™ flowsheet was designed to simulate the proposed HyS flowsheet discussed above. The flowsheet for each process condition is illustrated in Appendix A. The stream composition and conditions are detailed in Appendix B. The thermodynamic model used for these simulations was the OLI Systems Mixed Solvent Electrolyte (MSE) model. The model represents the H_2SO_4-H_2O system very well over its entire composition range. The MSE model represents the H_2SO_4-H_2O model accurately up to temperatures of 500℃. The d ecomposition section of the proposed HyS cycles was therefore simulated using the ELECTNRTL model provided by Aspen Plus™ due to its high temperature operating conditions of up to 870℃.

CHAPTER 4

RESULTS AND DISCUSSION:

TECHNICAL

4. Results and Discussion: Technical

Chapter 3 provided a detailed description of the execution of the designed HyS cycle. The analysis of the problem was executed using the engineering tool Aspen Plus^{TM} with OLI systems MSE model and ELECNRTL model.

Chapter 4 describes the flowsheet for each of the four cases that were investigated. The technical results calculated from the Aspen Plus^{TM} simulations such as the stream compositions and conditions will be tabulated within the chapter and will be discussed. The chapter will also include calculations on the mass and energy balances. The simulations are based on a HyS production plant that is linked to a 500MWt High Temperature Gas Reactor (HTGR) such as a PBMR.

Results from the simulations are technically evaluated to ensure accurate results were obtained. This is also discussed in chapter 4.

The purpose of this study is to firstly analyze and obtain technical results for various process conditions for a proposed HyS cycle. The technical evaluation includes a mass balance and energy balance which also provides the basis for calculating the raw material requirements, electricity consumption, process steam value, labour requirements, etc. Thereafter the results are evaluated to conduct an economic evaluation of each process condition thus determining the $/kg hydrogen production cost. The results from the technical and economic evaluation will be used to determine the operating range which will allow the HyS cycle to operate at profitable conditions. The technical evaluation's first step is to propose a HyS cycle flowsheet. It was simulated using the Aspen Plus^{TM} engineering tool.

4.1 Flowsheet

The operating conditions that have an effect on hydrogen production, energy consumption and the size of the plant were identified. Various operating conditions have been proposed. The factors identified include the pressure of the reactor section and the temperature of the sulphur trioxide reactor. The concentration of the sulphuric acid also play a role, however based on previous studies it was decided to make use of the optimal 80 mol% sulphuric acid feed to the decomposition reactor (Gorensek *et al.*, 2009:25).

Table 2 displays the operating conditions of the four different decomposition reactors that will be investigated in this study. Each of the cases was simulated making use of Aspen Plus^{TM} and the respective process flowsheets, mass and energy balances are given.

The rational behind the different cases chosen was to illustrate the influence of operating temperature and pressure on the conversion of the sulphuric acid and sulphur dioxide. This in turn has a potential influence on the water balance within the cycle, which will influence the energy input required to heat the water throughout the process.

Table 2: Operating conditions for flowsheet cases.

Temperature and Pressure Effect at 80 mol% Sulphuric Acid Concentration Feed				
Case	Sulphuric Acid Reactor Pressure (bar)	Sulphur Trioxide Reactor Pressure (bar)	Sulphuric Acid Reactor Temperature (ºC)	Sulphur Trioxide Reactor Temperature (ºC)
1	3	3	550	870
2	40	40	550	870
3	90	90	550	870
4	3	3	550	750

The process flowsheets for Cases 1, 2, 3 and 4 are illustrated in Figures 19 to 22 (as attached in Appendix A). The figures illustrate the proposed HyS for operating conditions stated in Table 2. The respective stream names and stream compositions are attached in Appendix B.

4.2 Mass Balance

The mass balance for each case is presented in tabulated form. The mass and energy balance done for the decomposition section was performed using manual calculations. The mass balance done for the decomposer section is attached in Appendix C. The mass balance that was done for the whole HyS was performed by making use of Aspen Plus^{TM} and is attached in Appendix B. A summary of the production rate of products and the unreacted reagents at the specified operating conditions are also discussed.

4.2.1 Case 1

The maximum production of hydrogen and oxygen (the by-product) which can be obtained at the operating conditions applicable to Case 1, are tabulated below in Table 3.

Table 3: Production rate of products and unreacted reagents for Case 1.

SO_3 production	
376.6	mol/s
30.2	kg/s
SO_2 production	
968.4	mol/s
62.0	kg/s
O_2 production	
484.2	mol/s
15.5	kg/s
H_2O production	
1682.5	mol/s
30.3	kg/s
H_2 production	
968.4	mol/s
1.95	kg/s
168.7	TPD
Conversion H_2SO_4	
0.996	
Conversion SO_3	
0.72	

A decomposition rate of 99.6% H_2SO_4 is obtained in the decomposer section and a conversion of SO_3 to SO_2 of 72% is achieved in reactor RX-102. The production rate of SO_2 in RX-102 is 968 mol/s which corresponds to a production rate of 968 mol/s of hydrogen. This is equivalent to a production rate of 1.96 kg/s hydrogen at 3 bar and 870℃ process conditions at which RX-102 is operate d. A total of 168.7 TPD of hydrogen production could be achieved for Case 1.

4.2.2 Case 2

The maximum production of hydrogen and oxygen, the co-product, which can be obtained at the operating conditions of Case 2 is tabulated below in Table 4.

Table 4: Production rate of products and unreacted reagents for Case 2.

SO_3 production	
605.0	mol/s
48.4	kg/s
SO_2 production	
710.0	mol/s
45.4	kg/s
O_2 production	
355.0	mol/s
11.4	kg/s
H_2O production	
1653.0	mol/s
29.8	kg/s
H_2 production	
710.0	mol/s
1.43	kg/s
123.7	TPD
Conversion H_2SO_4	
0.97	
Conversion SO_3	
0.54	

For Case 2 operating conditions a decomposition rate of 97% H_2SO_4 is obtained in the decomposer section and a conversion of SO_3 to SO_2 of 54% is achieved in reactor RX-102. The production rate of SO_2 in RX-102 is 710 mol/s and thus the production rate of 710 mol/s hydrogen is achieved. This amounts to a production rate of 1.43 kg/s hydrogen at 40 bar and 870℃ operating conditions for RX-102. A total of 123.7 TPD will be achievable for Case 2 operating conditions. A total of 11.4 kg/s oxygen are also being produced as a by-product.

4.2.3 Case 3

The maximum production of hydrogen and oxygen, the co-product, which can be obtained at the operating conditions of Case 3 is tabulated below in Table 5.

Table 5: Production rate of products and unreacted reagents for Case 3.

SO_3 production	
695.0	mol/s
55.6	kg/s
SO_2 production	
582.0	mol/s
37.2	kg/s
O_2 production	
291.0	mol/s
9.3	kg/s
H_2O production	
1615.0	mol/s
29.1	kg/s
H_2 production	
582.0	mol/s
1.17	kg/s
101.4	TPD
Conversion H_2SO_4	
0.95	
Conversion SO_3	
0.46	

For Case 3 operating conditions a decomposition rate of 95% H_2SO_4 is obtained in the decomposer section and a conversion of SO_3 to SO_2 of only 46% is achieved in reactor RX-102. The production rate of SO_2 in RX-102 is 582mol/s and thus the production rate of 582 mol/s hydrogen is achieved. This amounts to a production rate of 1.17 kg/s hydrogen at 90 bar and 870℃ operating conditions for RX-102. A total of 101.4 TPD will be achievable for Case 3 operating conditions. A total of 9.3 kg/s oxygen are also being produced as a by-product.

4.2.4 Case 4

The maximum production of hydrogen and oxygen, the co-product, which can be obtained at the operating conditions of Case 4 is tabulated below in Table 6.

Table 6: Production rate of products and unreacted reagents for Case 4.

SO_3 production	
590.0	mol/s
47.2	kg/s
SO_2 production	
752.0	mol/s
48.1	kg/s
O_2 production	
376.0	mol/s
12.0	kg/s
H_2O production	
1680.0	mol/s
30.2	kg/s
H_2 production	
752.0	mol/s
1.52	kg/s
131.0	TPD
Conversion H2SO4	
0.99	
Conversion SO3	
0.56	

A decomposition rate of 99% H_2SO_4 is obtained in the decomposer section and a conversion of SO_3 to SO_2 of 56% is achieved in reactor RX-102. The production rate of SO_2 in RX-102 is 752mol/s and thus the production rate of 752 mol/s hydrogen is achieved. This amounts to a production rate of 1.52kg/s hydrogen at 3 bar and 750℃ operating conditions for RX-102. A total of 131.0 TPD will be achievable for Case 4 operating conditions. A total of 12.0 kg/s oxygen are also being produced as a by-product.

4.2 Energy Balance

An energy balance for each of the cases 1 to 4 was done and tabulated within this section. The energy balance is also done to determine the electric power requirements of the cycle. The helium heat source provided by the HTGR is a maximum of 500 MWt heat. The required thermal heat is used by the decomposer system for the endothermic decomposition reactions and for the vaporization of the concentrated sulphuric acid stream. Thereafter the remaining heat, not utilized in the decomposer and vaporization section, is used for heating of streams throughout the cycle. An integrated heat exchanger system is used and it is assumed that the available heat is used efficiently (heat pinching). Electric power is required for the running of compressors, pumps, the cryogenic cooling system and the electrolyzer. This is tabulated on the right side of each of the respective energy balance tables.

The energy balances are conducted by adding up the total thermal energy requirement of the process and the electrical energy requirement. The electrical energy requirement is then converted to thermal energy units. The conversion factor from thermal power to electric power has been assumed to be 40% efficient. The value obtained from adding the thermal and electrical energy requirements indicates whether electricity will be imported or exported. 500 MWt is used as the basis.

Table 7 provides the results for Case 1 operating conditions.

Table 7: Energy Balance Case 1.

Unit Operation (Thermal Heat)	MW	Unit Operation (Electricity)	MW
HX-101	22.22	PP-101	0.01
HX-102	5.20	PP-102	0.02
HX-103	136.78	PP-103	0.00
EX-101	0	PP-104	0.01
RX-101	38.69	PP-105	0.08
EX-102	0	CO-101	35.31
RX-102	120.94	CO-102	17.10
HX-104	-52.77	CO-103	0.17
HX-105	-57.00	CO-104	8.37
HX-106	-135.88	Cryogenic - HX-110	5.85
HX-107	-17.54	Electrolyzer	117.0
HX-108	-12.60		
HX-109	-118.34		
HX-111	17.54		
HX-112	73.10		
HX-113	-1.75		
HX-114	-1.65		
HX-115	1.86		
HX-116	21.03		
HX-117	-0.91		
HX-118	-18.25		
HX-119	-0.00		
HX-120	8.91		
HX-121	-0.12		
HX-122	-0.11		
HX-123	-3.35		
HX-124	-0.13		
HX-125	-3.19		
HX-126	-9.70		
HX-127	132.10		
HX-128	-3.29		
HX-129	-6.89		
HX-130	-25.45		
HX-131	-0.04		
HX-132	-0.02		
HX-133	-0.02		
HX-134	-0.08		
HX-135	0.10		
HX-136	0.46		
DR-101	-0.41		
DR-102	-0.16		
Hydrogen Production Rate (kg/s)			**1.94**
Process Heat from Nuclear Reactor (MWt)			**500**
HYS Thermal Heat Requirement (MW)			**296.41**
HYS Electrical Requirement (MW)			**183.88**
Thermal Equivalent of Electric input (MW) @ 40 % Conversion Efficiency			459.70
Total Heat Input (MW)			**756.11**
Surplus Process Heat For Electricity Generation (MW)			0.00
Electricity Import (MW) @ 40% Conversion Efficiency			**102.44**
Lower Heating Value of Hydrogen (MJ/kg)			120.00
Higher Heating Value of Hydrogen (MJ/kg)			144.00
Lower Heating Equivalent of Produced Hydrogen (MW)			232.41
Higher Heating Equivalent of Produced Hydrogen (MW)			278.90
Thermal Efficiency (Lower Heating Value) %			**30.74**
Thermal Efficiency (Higher Heating Value) %			**36.89**

The operating conditions of Case 1 require an electricity import of 102.44 MW. The units that mainly contribute to the electricity requirements within the HyS cycle are the compressor within the separation section and the electrolyzer. The reason for a high compressor power requirement within the separation section is due to the low pressure conditions within the reactors and the volume of the stream that needs to be compressed. In case of low pressure conditions the product stream from the reactor section will require compression to obtain a stream condition of 20 bar at which the separation between SO_2/O_2 are performed.

In the case of the electrolyzer, the energy requirements are high due to a high hydrogen production rate. The effect of the volume of hydrogen produced will be illustrated in the following cases where the hydrogen production rate varies. The electrolyzer is an expensive operation and is responsible for most of the electricity consumption.

A factor that influences the electricity use within an electrolyzer is the standard cell voltage. This is the minimum amount of electricity require to split the water into hydrogen and oxygen. A higher concentration of sulphuric acid increases this value. At 50wt% sulphuric acid the standard cell voltage is 0.243V and this increases as the concentration increases which in turn will increase the amount the electricity used by the electrolyzer.

Table 8 gives the results for Case 2 operating conditions.

Table 8: Energy Balance Case 2.

Unit Operation (Thermal Heat)	MW	Unit Operation (Electricity)	MW
HX-101	22.23	PP-101	6.78
HX-102	5.20	PP-102	0.31
HX-103	155.43	PP-103	0.00
EX-101	0	PP-104	0.01
RX-101	38.02	PP-105	0.66
EX-102	48	CO-101	38.81
RX-102	69.82	CO-102	14.70
HX-104	-110.67	CO-103	0.11
HX-105	-59.52	CO-104	10.22
HX-106	-145.85	Cryogenic - HX-110	5.38
HX-107	-28.86	Electrolyzer	81.6
HX-108	-15.85		
HX-109	-117.77		
HX-111	17.20		
HX-112	124.96		
HX-113	-0.29		
HX-114	-1.21		
HX-115	0.37		
HX-116	4.06		
HX-117	-0.67		
HX-118	-20.94		
HX-119	-0.00		
HX-120	8.53		
HX-121	-3.99		
HX-122	-2.48		
HX-123	-2.48		
HX-124	-		
HX-125	-		
HX-126	-14.05		
HX-127	150.43		
HX-128	-4.02		
HX-129	-6.88		
HX-130	-25.45		
HX-131	-0.02		
HX-132	-0.01		
HX-133	-0.01		
HX-134	-0.06		
HX-135	-0.62		
HX-136	1.64		
DR-101	-0.30		
DR-102	-0.12		

Hydrogen Production Rate (kg/s)	**1.42**
Process Heat from Nuclear Reactor (MWt)	**500**
HYS Thermal Heat Requirement (MW)	**311.49**
HYS Electrical Requirement (MW)	**158.62**
Thermal Equivalent of Electric input (MW) @ 40 % Conversion Efficiency	396.56
Total Heat Input (MW)	**708.04**
Surplus Process Heat For Electricity Generation (MW)	0.00
Electricity Import (MW) @ 40% Conversion Efficiency	**83.22**
Lower Heating Value of Hydrogen (MJ/kg)	120.00
Higher Heating Value of Hydrogen (MJ/kg)	144.00
Lower Heating Equivalent of Produced Hydrogen (MW)	170.40
Higher Heating Equivalent of Produced Hydrogen (MW)	204.48
Thermal Efficiency (Lower Heating Value) %	**24.07**
Thermal Efficiency (Higher Heating Value) %	**28.88**

The operating conditions of Case 2 require an electricity import of 83.22 MW. The units that mainly contribute to the electricity requirements within the HyS cycle are the compressor within the separation section and the electrolyzer. It can be seen that the compressor requires more power than in Case 1 although the pressure in the reactors are higher. This could be due to the high gas volume that has to be compressed.

In the case of the electrolyzer the energy requirements are lower compared to Case 1 due to a lower hydrogen production rate.

Table 9 gives the results for Case 3 operating conditions.

Table 9: Energy Balance Case 3.

Unit Operation (Thermal Heat)	MW	Unit Operation (Electricity)	MW
HX-101	22.44	PP-101	0.63
HX-102	4.99	PP-102	19.99
HX-103	172.06	PP-103	0.00
EX-101	0	PP-104	0.01
RX-101	4.16	PP-105	0.67
EX-102	42	CO-101	35.11
RX-102	80.79	CO-102	12.53
HX-104	-143.05	CO-103	0.09
HX-105	-60.05	CO-104	10.65
HX-106	-144.11	Cryogenic - HX-110	4.70
HX-107	-27.39	Electrolyzer	65.2
HX-108	-14.32		
HX-109	-105.54		
HX-111	15.29		
HX-112	127.84		
HX-113	-0.08		
HX-114	-0.99		
HX-115	0.15		
HX-116	3.41		
HX-117	-0.56		
HX-118	-18.85		
HX-119	-0.00		
HX-120	7.65		
HX-121	-4.68		
HX-122	-2.91		
HX-123	-11.04		
HX-124	-		
HX-125	-		
HX-126	-16.49		
HX-127	154.54		
HX-128	-4.19		
HX-129	-6.86		
HX-130	-25.36		
HX-131	-0.02		
HX-132	-0.01		
HX-133	-0.01		
HX-134	-0.05		
HX-135	-0.64		
HX-136	1.67		
DR-101	-0.25		
DR-102	-0.10		

Hydrogen Production Rate (kg/s)	**1.16**
Process Heat from Nuclear Reactor (MWt)	**500**
HYS Thermal Heat Requirement (MW)	**299.23**
HYS Electrical Requirement (MW)	**149.64**
Thermal Equivalent of Electric input (MW) @ 40 % Conversion Efficiency	374.11
Total Heat Input (MW)	**673.34**
Surplus Process Heat For Electricity Generation (MW)	0.00
Electricity Import (MW) @ 40% Conversion Efficiency	**69.34**
Lower Heating Value of Hydrogen (MJ/kg)	120.00
Higher Heating Value of Hydrogen (MJ/kg)	144.00
Lower Heating Equivalent of Produced Hydrogen (MW)	139.68
Higher Heating Equivalent of Produced Hydrogen (MW)	167.62
Thermal Efficiency (Lower Heating Value) %	**20.74**
Thermal Efficiency (Higher Heating Value) %	**24.89**

The operating conditions of Case 3 require an electricity import of 69.34 MW. The units that mainly contribute to the electricity requirements within this HyS cycle are the compressor within the separation section and the electrolyzer.

In the cases of the electrolyzer the energy requirements are lower compared to Case 1 and Case 2 due to a lower hydrogen production rate.

Table 10 gives the results for Case 4 operating conditions.

Table 10: Energy Balance Case 4.

Unit Operation (Thermal Heat)	MW	Unit Operation (Electricity)	MW
HX-101	22.22	PP-101	5.77
HX-102	5.20	PP-102	12.03
HX-103	135.73	PP-103	0.00
EX-101	35.57	PP-104	0.01
RX-101	66.91	PP-105	0.29
EX-102	7	CO-101	28.58
RX-102	74.39	CO-102	14.20
HX-104	-114.56	CO-103	0.13
HX-105	-60.37	CO-104	10.71
HX-106	-150.07	Cryogenic - HX-110	4.62
HX-107	-15.10	Electrolyzer	89.4
HX-108	-10.05		
HX-109	-94.33		
HX-111	13.93		
HX-112	78.91		
HX-113	-0.02		
HX-114	-1.28		
HX-115	0.11		
HX-116	19.98		
HX-117	-0.71		
HX-118	-17.34		
HX-119	-0.00		
HX-120	7.10		
HX-121	-0.18		
HX-122	-0.17		
HX-123	-4.94		
HX-124	-0.19		
HX-125	-4.79		
HX-126	-14.59		
HX-127	155.34		
HX-128	-4.21		
HX-129	-6.89		
HX-130	-25.48		
HX-131	-0.03		
HX-132	-0.01		
HX-133	-0.01		
HX-134	-0.06		
HX-135	-0.02		
HX-136	1.16		
DR-101	-0.32		
DR-102	-0.12		

Hydrogen Production Rate (kg/s)	**1.50**
Process Heat from Nuclear Reactor (MWt)	**500**
HYS Thermal Heat Requirement (MW)	**319.51**
HYS Electrical Requirement (MW)	**165.72**
Thermal Equivalent of Electric input (MW) @ 40 % Conversion Efficiency	414.31
Total Heat Input (MW)	**733.82**
Surplus Process Heat For Electricity Generation (MW)	0.00
Electricity Import (MW) @ 40% Conversion Efficiency	**93.53**
Lower Heating Value of Hydrogen (MJ/kg)	120.00
Higher Heating Value of Hydrogen (MJ/kg)	144.00
Lower Heating Equivalent of Produced Hydrogen (MW)	180.48
Higher Heating Equivalent of Produced Hydrogen (MW)	216.58
Thermal Efficiency (Lower Heating Value) %	**24.59**
Thermal Efficiency (Higher Heating Value) %	**29.51**

The operating conditions of Case 4 require an electricity import of 93.53 MW. The units that mainly contribute to the electricity requirements within this HyS cycle are the compressor within the separation section and the electrolyzer.

In the case of the electrolyzer the energy requirements are higher compared to Case 2 and 3 but lower than Case 1 due to a lower hydrogen production rate.

4.3 Electrolyzer

The electrolyzer is the main contributor to the electrical consumption of the proposed HyS cycle. The electric power requirement for the electrolysis of water in the presence of SO_2 will range from 117 MW to 65 MW for the various process operating conditions under investigation. The calculation of the electric power requirement of an electrolyzer is based on the operating cell voltage and the current density. To calculate the power usage of the electrolyzer the following parameters must be established:

- The acid concentration at the electrolyzer outlet.
- The amount of SO_2 dissolved (use the saturation value).
- The reversible potential.

The reversible potential calculations are detailed in Appendix D. The next step is to determine the overpotential. The overpotential for the electrolyzer can only be determined by practical experimentation. Therefore an educated estimation of the overpotential value is used for this study. The value is based on overpotential values used by SRNL. For this study it was estimated to be 0.3V. The overpotential is then added to the reversible potential to calculate the cell voltage. The following step is to calculate the current using Faraday's law. The electric power requirements of the electrolyzer are obtained by multiplying the cell voltage by the value of the current.

The calculations of the reversible potential are done by means of the Nernst Equation.

$$E = E^0 - \frac{RT}{nF} \ln Q$$

where

$$Q = \frac{(a_{SO_2})(a_{H_2O})^2}{[(a_{SO_4^-})(a_{H_2})(10^{-2pH})]}$$

Supporting documentation for the reversible potential calculation is attached in Appendix D.

The calculation of the current is executed and obtained by means of using Faraday's law. The first law of Faraday of electrolysis is that the quantity of a substance produced by electrolysis is proportional to the quantity of electricity being used. Faraday constant, F, is the quantity of electricity carried by one mole of electrons.

$$F = N_A \cdot \text{charge of electron}$$

$$F = 6.022 \times 10^{23} mol^{-1} \cdot 1.602192 x 10^{-19} C$$

The quantity of electricity required to electrolyze water can be determined by:

$$Q = n(e) \times F$$

The electrical energy is calculated by:

$$E = Q \times V$$

The electrolyzer electric power requirements for Case 1 are tabulated in Table 11. The reversible potential calculations are detailed in Appendix D. For this study the overpotential is estimated to be 0.3V.

Table 11: Case 1 Electrolyzer calculations.

H_2 produced	0.968	kmol/s
H_2SO_4 wt%	56	wt%
Reversible Potential	0.326	Volt
Overpotential Estimate	0.3	Volt
$SO_2 + 2H_2O$? $H_2SO_4 + 2H^+ + 2e^-$		
FOR 1 kmol		
1 Amp = 1 C/s		
$1e^- = 1.602 \times 10^{-19}$ C		
1 mole of electron = 6.022×10^{23} electrons		
Electrolyzer current	192944880	C/s for 1kmol
	186846799	C/s for 0.968kmol
Electrolyzer power consumption	116966096	W
Electrolyzer power consumption	**117**	**MW**

For Case 1 the electrolyzer has a reversible potential of 0.326V and a total cell voltage of 0.626V. The total electric power consumption for Case 1 electrolyzer is 117MW.

The electrolyzer electric power requirements for Case 2 are tabulated in Table 12. The reversible potential calculations are detailed in Appendix D. For this study the overpotential is estimated to be 0.3V.

Table 12: Case 2 Electrolyzer calculations.

H_2 produced	0.710	kmol/s
H_2SO_4 wt%	50	wt%
Reversible Potential	0.296	Volt
Overpotential Estimate	0.3	Volt
$SO_2 + 2H_2O$? $H_2SO_4 + 2H^+ + 2e^-$		
FOR 1 kmol		
1 Amp = 1 C/s		
$1e^- = 1.602 \times 10^{-19}$ C		
1 mole of electron = 6.022×10^{23} electrons		
Electrolyzer current	192944880	C/s for 1kmol
	136990865	C/s for 0.710kmol
Electrolyzer power consumption	81646555	Watt
Electrolyzer power consumption	82	MW

For Case 2 the electrolyzer has a reversible potential of 0.296V and a total cell voltage of 0.596V. The total electric power consumption for Case 2 electrolyzer is 82MW.

The electrolyzer electric power requirements for Case 3 are tabulated in Table 13. The reversible potential calculations are detailed in Appendix D.

Table 13: Case 3 Electrolyzer calculations.

H_2 produced	0.582	kmol/s
H_2SO_4 wt%	47	wt%
Reversible Potential	0.281	Volt
Overpotential Estimate	0.3	Volt
$SO_2 + 2H_2O$? $H_2SO_4 + 2H^+ + 2e^-$		
FOR 1 kmol		
1 Amp = 1 C/s		
$1e^- = 1.602 \times 10^{-19}$ C		
1 mole of electron = 6.022×10^{23} electrons		
Electrolyzer current	192944880	C/s for 1kmol
	112293920	C/s for 0.582 kmol
Electrolyzer power consumption	65242767.6	W
Electrolyzer power consumption	**65**	**MW**

For Case 3 the electrolyzer has a reversible potential of 0.281V and a total cell voltage of 0.581V. The total electric power consumption for Case 3 electrolyzer is 65MW.

The electrolyzer electric power requirements for Case 4 are tabulated in Table 14. The reversible potential calculations are detailed in Appendix D.

Table 14: Case 4 Electrolyzer calculations.

H_2 produced	0.752	kmol/s
H_2SO_4 wt%	54	wt%
Reversible Potential	0.316	Volt
Overpotential Estimate	0.3	Volt
$SO_2 + 2H_2O$? $H_2SO_4 + 2H^+ + 2e^-$		
FOR 1 kmol		
1 Amp = 1 C/s		
$1e^- = 1.602 \times 10^{-19}$ C		
1 mole of electron = 6.022×10^{23} electrons		
Electrolyzer current	192,944,880	C/s for 1kmol
	145,094,550	C/s for 0.752 kmol
Electrolyzer power consumption	89378242.65	W
Electrolyzer power consumption	**89**	**MW**

For Case 4 the electrolyzer has a reversible potential of 0.316V and a total cell voltage of 0.616V. The total electric power consumption for Case 4 electrolyzer is 89 MW.

4.4 Discussion

The proposed HyS cycle technical evaluation was preformed using the engineering tool Aspen PlusTM. The models used for the simulation task were ELECTNRTL and OLI MSE. Both these models were chosen based on their ranges and limits that best fits the proposed HyS cycle. The proposed HyS cycle do require optimization of the thermal heat use and the layout of the plant.

The results from the technical evaluation indicate that operating at low pressures and high temperatures will result in high conversions and production rates. However, operating at these conditions affects the energy consumption of the cycle. The energy balance was done to investigate the effect of various operating conditions with various conversion efficiencies on the energy consumption of the cycle. For higher conversion of H_2SO_4 and SO_3, resulting in a higher production rate of hydrogen, the total amount of energy import is higher than for lower conversion of H_2SO_4 and SO_3.

The thermal efficiency of each cycle was also calculated. For the lower operating pressures and high temperatures the thermal efficiency of the Lower Heating Values (LHV) and the Higher Heating Values (HHV) are higher than those operating at higher pressures. Figure 14 indicates the highest thermal efficiencies could be obtained for Case 1.

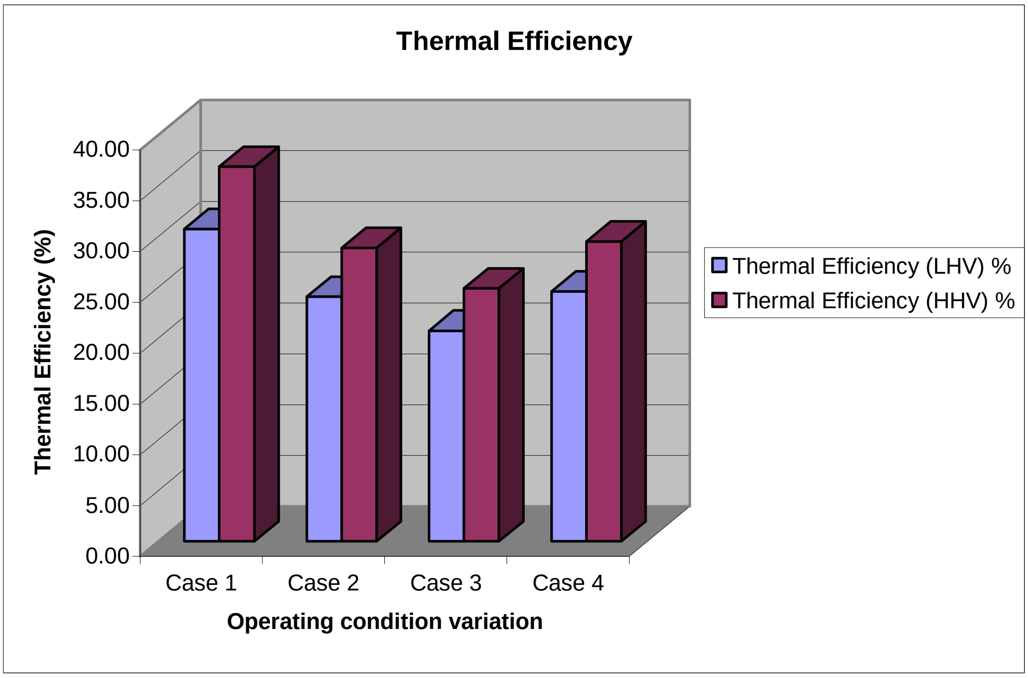

Figure 14: Thermal Efficiency for various operating conditions.

CHAPTER 5

RESULTS AND DISCUSSION: ECONOMIC

5. Results and Discussion: Economic

Chapter 4 gives a presentation and discussion on the technical results of the proposed solution to the HyS investigation. The technical evaluation includes the proposed HyS flowsheet simulated in Aspen Plus^{TM}. The chapter also contains the results of the mass balance of each of the four investigated operating conditions, tabulating the hydrogen and oxygen production rates as well as the unreacted reagents flow rates. The energy balance is presented in Chapter 4 which included the results of the electricity import or export requirements at the proposed operating conditions. The cycle thermal efficiency was also calculated from the energy balance of the cycle for each of the operating conditions. The energy balance could only be performed when the electrolyzer electric power requirements are known. The chapter also briefly discussed the method of the electrolyzer electricity calculation.

Chapter 5 will make use of the technical results to determine the economic implications that each of the four operating conditions will have on the cost of hydrogen production. In this chapter the variable costs (water, electricity, nuclear heat, etc.) and fixed costs (maintenance and repair, labour, etc.) for the production of H_2 will be calculated for each of the cycles. A sensitivity analysis will also indicate which variable and fixed cost factors will have the biggest impact on the cost of hydrogen production.

5.1 Economic model

To determine the cost to produce a specified product one needs to develop a cost estimation of the proposed process plant. This entails the calculation of the capital required for the fixed capital investment (FCI) and the working capital investment (WCI). The fixed capital investment, also called the CAPEX, consists of two sections namely the direct costs and the indirect costs. The CAPEX components are tabulated below in Table 15 (Peters *et al.*, 2003:240).

Table 15: FCI components (Peters *et al.*, 2003).

Component	Range of FCI %
Direct Costs	
Purchased equipment	15-40
Purchased-equipment installation	6-14
Instrumentation and Controls (Installed)	2-12
Piping (Installed)	4-17
Electrical systems (Installed)	2-10
Buildings (Including services)	2-18
Yard improvements	2-5
Service facilities (Installed)	8-30
Land	1-2
Indirect Costs	
Engineering and supervision	4-20
Construction expenses	4-17
Legal expenses	1-3
Contractor's fee	2-6
Contingency	5-15

The working capital consists of two sections, being variable costs and fixed costs. The variable costs are costs for supplying raw material and other operating expenses such as electricity, nuclear heat supply, catalyst and water. The variable costs are the costs associated with the manufacturing process, meaning it is the costs that will vary with the variation in hydrogen production rate. The fixed costs include costs for labor, insurance, maintenance and repairs. These costs are independent of the production rate. The sum of the FCI and WC delivers the Total Capital Investment (TCI).

A sensitivity model is executed, which will allow the study to determine which factor will have the most significant influence on the cost of hydrogen production.

5.1.1 Assumptions for this economic model

- CEPCI June 2009 = 508.9 (CHE, 2009:64).
- CEPCI 2008 = 575.4 (CHE, 2009:64).
- Oxygen selling price is $40 per ton (as a credit).
- Plant life time – 40 years.
- Plant availability – 94%.

5.2 Fixed Capital Investment

The capital cost estimation for the HyS is based on *the order-of-magnitude estimate (ratio estimate)* method. This method is based on the availability of similar cost data for a similar process plant. The probable accuracy of this method is more than 30 percent.

In case of the use of the order-of-magnitude estimate method one has to adapt the values for the present time as most preliminary estimates are only valid for the time they were developed. The use of cost indexes was developed to adapt the values to present values. The chemical engineering plant cost indexes (CEPCI) were used to present accurate CAPEX values for a HyS processing plant. The method used to adapt the values is:

$$\text{Present cost} = \text{original cost}\left(\frac{\text{CEPCI at present}}{\text{CEPCI at time original cost was obtained}}\right)$$

The order-of-magnitude method uses the FCI of a similar previously constructed plant to estimate the FCI of a new process plant by means of an exponential power ratio. The FCI for the new process plant is determined by (Peters *et al.*, 2003:254):

$$C_n = C f_e R^x$$

where:

C_n = FCI of the new facility,

R = capacity of new facility divided by the capacity of the old facility,

C = FCI of the old facility,

f_e = cost index ratio, and

x = power equal to 0.6 or 0.7.

The CEPCI for 2008 was 575.4 and for June 2009 it was calculated as 508.9 (CHE, 2009:64). These values were used for the economic modelling and determination of the Fixed Capital Investment.

Tables 16-19 contain the equipment and direct costs of the reference HyS cycle (Gorensek *et al.*, 2009:76), excluding the NHSS, BOP and PGS. The tables also provide the calculated FCI for the proposed HyS, calculated by the method discussed above. The FCI values for Cases 1, 2, 3 and 4 are tabulated below.

Table 16: FCI for Case 1.

EQUIPMENT & DIRECT COSTS CAPEX	Reference HyS (Gorensek et al., 2009:76)	Proposed HyS
Electrolyzer	$174,800,000	$153,715,483
Reactor, Concentration, Separation	$206,000,000	$181,152,114
Water Treatment	$16,600,000	$14,597,695
Purification	$62,300,000	$54,785,324
Total direct plant cost	**$459,700,000**	$404,250,615
EPC fee at 5%	**$22,985,000**	$20,212,531
TOTAL DIRECT COSTS	$482,685,000	$424,463,146
TOTAL INDIRECT COST		$127,338,944
CONTINGENCY		$42,446,315
FIXED CAPITAL INVESTMENT		$594,248,404
OPERATING COST VARIABLE		**$212,566,967**
OPERATING COST FIXED		**$36,198,864**
TOTAL PRODUCTION COST		**$843,014,235**

Table 17: FCI for Case 2.

EQUIPMENT & DIRECT COSTS CAPEX	Reference HyS (Gorensek et al., 2009:76)	Proposed HyS
Electrolyzer	$174,800,000	$127,586,142
Reactor, Concentration, Separation	$206,000,000	$150,358,955
Water Treatment	$16,600,000	$12,116,304
Purification	$62,300,000	$45,472,635
Total direct plant cost	**$459,700,000**	$335,534,036
EPC fee at 5%	**$22,985,000**	$16,776,702
TOTAL DIRECT COSTS	$482,685,000	$352,310,738
TOTAL INDIRECT COST		$105,693,221
CONTINGENCY		$35,231,074
FIXED CAPITAL INVESTMENT		$493,235,034
OPERATING COST VARIABLE		**$197,342,277**
OPERATING COST FIXED		**$30,138,062**
TOTAL PRODUCTION COST		**$720,715,373**

Table 18: FCI for Case 3.

EQUIPMENT & DIRECT COSTS CAPEX	Reference HyS (Gorensek et al., 2009:76)	Proposed HyS
Electrolyzer	$174,800,000	$113,242,486
Reactor, Concentration, Separation	$206,000,000	$133,455,103
Water Treatment	$16,600,000	$10,754,149
Purification	$62,300,000	$40,360,451
Total direct plant cost	**$459,700,000**	$297,812,190
EPC fee at 5%	**$22,985,000**	$14,890,609
TOTAL DIRECT COSTS	$482,685,000	$312,702,799
TOTAL INDIRECT COST		$93,810,840
CONTINGENCY		$31,270,280
FIXED CAPITAL INVESTMENT		$437,783,919
OPERATING COST VARIABLE		**$186,901,814**
OPERATING COST FIXED		**$26,810,995**
TOTAL PRODUCTION COST		**$651,496,728**

Table 19: FCI for Case 4.

EQUIPMENT & DIRECT COSTS CAPEX	Reference HyS (Gorensek et al., 2009:76)	Proposed HyS
Electrolyzer	$174,800,000	$132,049,024
Reactor, Concentration, Separation	$206,000,000	$155,618,415
Water Treatment	$16,600,000	$12,540,125
Purification	$62,300,000	$47,063,239
Total direct plant cost	**$459,700,000**	$347,270,803
EPC fee at 5%	**$22,985,000**	$17,363,540
TOTAL DIRECT COSTS	$482,685,000	$364,634,343
TOTAL INDIRECT COST		$109,390,303
CONTINGENCY		$36,463,434
FIXED CAPITAL INVESTMENT		$510,488,081
OPERATING COST VARIABLE		**$204,054,806**
OPERATING COST FIXED		**$31,173,245**
TOTAL PRODUCTION COST		**$745,716,131**

A contingency of 10% of the total direct costs was applied for this study (Gorensek *et al.*, 2009:73). An indirect cost of 30% of the direct costs, were applied which include engineering, legal fees and contractors fees.

5.3 Working capital variable costs

The variable costs are dependent on the production rate of the processing plant. The costs include the expenditure for raw materials, chemicals, catalyst, replacements of filters and tubes, and cost of utilities. The utilities may include cooling water for coolers, process steam for the vacuum operation, process water for purification purposes, processing, softening and RO/EDI, and also electricity costs. The values for these variable costs calculations were obtained from the simulations done by making use of Aspen Plus^{TM} except for the process water for purification, softening and RO/EDI, replacement costs and catalyst costs. These functions were not simulated within the Aspen Plus^{TM} simulations, but were obtained from a previous similar study (Bolthrunis, 2009:Section 8.1.8). The scaling method was used for determining the quantities required for the size of the plant.

The costs per quantity of the utilities, except for the electricity cost, were determined by calculations as suggested by Ulrich and Vasudevan (2006:66-69). Ulrich and Vasudevan suggest an approach which uses a two-factor utility cost equation and relevant coefficient for estimating the utility costs. The approach is based on the dependency of utilities on inflation and energy costs.

The variable costs for Cases 1 to 4 are given in Tables 20 - 23 respectively.

5.4 Working capital fixed costs

The fixed costs are the costs that are independent from the production rate of the process plant. The fixed costs for the HyS include maintenance and repairs, operating labor, overhead costs, insurance and nuclear heat.

The labour basic hourly rate of $50 average is applied. The overhead costs are included in the operating labour calculations at 20% of the labour rate. The total operating labor and overhead costs amounts to $60/hour.

An insurance cost of 1% of the fixed capital investment and maintenance and repairs of 5% of FCI is applied. The nuclear heat costs have been assumed as $30 per MWt (Bolthrunis, 2009:Section 8.1.8).

The fixed costs for Cases 1 to 4 are also given in Tables 20 - 23 respectively.

Table 20: Variable and Fixed Costs for Case 1.

Hybrid Sulphur Cycle Case 1		Date	2009	
Pressure	3bar	CEPCI	508.9	
SO_3 Reactor Temperature	870°C			
Capacity TPD	159			
Product:	H_2	Capacity (kg/h):	7,029.24	
Operating time (h/yr):	8234.4	Capacity (kg/s):	1.95	
Capacity (kg/yr):	57881554.1	Fixed Capital Investmen	$594,248,404	
	Quantity per year	Cost per quanitity	Unit	Cost per year
VARIABLE COSTS				
Raw Materials				
H2SO4 (ton)	428	115	$/ton	$49,265
Sulphur Trioxide tubes		218	$/hr	$1,761,579
Electrolyzer refurbishment		359	$/hr	$2,901,424
Electrolyzer cell replacements		940.8	$/hr	$7,613,337
Filter replacement		66	$/hr	$536,862
Make-up catalyst (Decomposer)		260	$/hr	$2,104,026
ZnO		180	$/hr	$1,458,319
Mol Sieve		81	$/hr	$659,194
Hydrogenation catalyst		20	$/hr	$157,802
Make-up Acid	0.00	115	$/ton	$0.02651
Caustic (ton)	12994	385	$/ton	$4,916,380
Utilities				
Cooling Water	661,650,509	0.005	$/m^3	$3,070,550
Process Water				
Natural	515,120	0.072	$/m^3	$37,325
Softening	1311854	0.065	$/m^3	$85,050
RO/EDI	1039884	0.066	$/m^3	$68,933
Process Steam	4695584	0.077	$/kg	$363,555
Electricity	1514141	75	$/Mwe-h	$113,560,610
Heat	2440758.504	30	$/MWt-h	$73,222,755
			TOTAL VARIABLE COSTS	**$212,566,967**
FIXED COSTS				
Maintenance and Repair				$29,712,420
Operating labour + Over head = (20% of labour)				
	Operation - 4 per shift x 4shifts	60	$/hr	$350,400
	Maintenance - 2 per shift x 4 shifts + 6 day shift only	60	$/hr	$149,760
	1 Supervision per shift + 1 maintenance supervision	60	$/hr	$43,800
Insurance	1% of fixed capital			$5,942,484
			TOTAL FIXED COSTS	**$36,198,864**
			TOTAL PRODUCTION COSTS	**$248,765,831**

Table 21: Variable and Fixed Costs for Case 2.

Hybrid Sulphur Cycle Case 2		Date	2009	
Pressure	40bar	CEPCI	508.9	
SO_3 Reactor Temperature	870℃			
Capacity TPD	116			
Product:	H_2	Capacity (kg/h):	5,152.90	
Operating time (h/yr):	8234.4	Capacity (kg/s):	1.43	
Capacity (kg/yr):	42431006.8	Fixed Capital Investmen	$493,235,034	
	Quantity per year	Cost per quanitity	Unit	Cost per year
VARIABLE COSTS				
Raw Materials				
H2SO4 (ton)	477	115	$/ton	$54,816
Sulphur Trioxide tubes		218	$/hr	$1,459,524
Electrolyzer refurbishment		359	$/hr	$2,403,922
Electrolyzer cell replacements		940.8	$/hr	$6,307,892
Filter replacement		66	$/hr	$444,807
Make-up catalyst (Decomposer)		260	$/hr	$1,743,253
ZnO		180	$/hr	$1,208,264
Mol Sieve		81	$/hr	$546,163
Hydrogenation catalyst		20	$/hr	$130,744
Make-up Acid	0.00	115	$/ton	$0.00000
Caustic (ton)	12994	385	$/ton	$4,073,378
Utilities				
Cooling Water	794,158,474	0.005	$/m^3	$3,685,485
Process Water				
Natural	379,000	0.072	$/m^3	$27,462
Softening	958814	0.065	$/m^3	$62,161
RO/EDI	760035	0.066	$/m^3	$50,382
Process Steam	3041458	0.077	$/kg	$235,485
Electricity	1306141	75	$/Mwe-h	$97,960,540
Heat	2564933	30	$/MWt-h	$76,947,998
			TOTAL VARIABLE COSTS	**$197,342,277**
FIXED COSTS				
Maintenance and Repair				$24,661,752
Operating labour + Over head = (20% of labour)				
	Operation - 4 per shift x 4shifts	60	$/hr	$350,400
	Maintenance - 2 per shift x 4 shifts + 6 day shift only	60	$/hr	$149,760
	1 Supervision per shift + 1 maintenance supervision	60	$/hr	$43,800
Insurance	1% of fixed capital			$4,932,350
			TOTAL FIXED COSTS	**$30,138,062**
			TOTAL PRODUCTION COSTS	**$227,480,339**

Table 22: Variable and Fixed Costs for Case 3.

Hybrid Sulphur Cycle Case 3		Date	2009	
Pressure	90bar	CEPCI	508.9	
SO_3 Reactor Temperature	870℃			
Capacity TPD	95			
Product:	H_2	Capacity (kg/h):	4,224.04	
Operating time (h/yr):	8234.4	Capacity (kg/s):	1.17	
Capacity (kg/yr):	34782421.8	Fixed Capital Investmen	$437,783,919	
	Quantity per year	Cost per quanitity	Unit	Cost per year
VARIABLE COSTS				
Raw Materials				
H2SO4 (ton)	477	115	$/ton	$54,816
Sulphur Trioxide tubes		218	$/hr	$1,295,440
Electrolyzer refurbishment		359	$/hr	$2,133,666
Electrolyzer cell replacements		940.8	$/hr	$5,598,738
Filter replacement		66	$/hr	$394,801
Make-up catalyst (Decomposer)		260	$/hr	$1,547,270
ZnO		180	$/hr	$1,072,427
Mol Sieve		81	$/hr	$484,762
Hydrogenation catalyst		20	$/hr	$116,045
Make-up Acid	0.00	115	$/ton	$0.00000
Caustic (ton)	12994	385	$/ton	$3,615,435
Utilities				
Cooling Water	849,296,016	0.005	$/m^3	$3,941,365
Process Water				
Natural	309,605	0.072	$/m^3	$22,434
Softening	785978	0.065	$/m^3	$50,956
RO/EDI	623032	0.066	$/m^3	$41,300
Process Steam	2561228	0.077	$/kg	$198,303
Electricity	1232196	75	$/Mwe-h	$92,414,671
Heat	2463979.512	30	$/MWt-h	$73,919,385
			TOTAL VARIABLE COSTS	**$186,901,814**
FIXED COSTS				
Maintenance and Repair				$21,889,196
Operating labour + Over head = (20% of labour)				
	Operation - 4 per shift x 4shifts	60	$/hr	$350,400
	Maintenance - 2 per shift x 4 shifts + 6 day shift only	60	$/hr	$149,760
	1 Supervision per shift + 1 maintenance supervision	60	$/hr	$43,800
Insurance	1% of fixed capital			$4,377,839
			TOTAL FIXED COSTS	**$26,810,995**
			TOTAL MANUFACTURING COSTS	**$213,712,809**

Table 23: Variable and Fixed Costs for Case 4.

Hybrid Sulphur Cycle Case 4		Date	2009	
Pressure	3bar	CEPCI	508.9	
SO_3 Reactor Temperature	750℃			
Capacity TPD	123			
Product:	H_2	Capacity (kg/h):	5,456.79	
Operating time (h/yr):	8234.4	Capacity (kg/s):	1.52	
Capacity (kg/yr):	44933421.2	Fixed Capital Investmen	$510,488,081	
	Quantity per year	Cost per quanitity	Unit	Cost per year
VARIABLE COSTS				
Raw Materials				
H2SO4 (ton)	477	115	$/ton	$54,816
Sulphur Trioxide tubes		218	$/hr	$1,513,281
Electrolyzer refurbishment		359	$/hr	$2,492,464
Electrolyzer cell replacements		940.8	$/hr	$6,540,224
Filter replacement		66	$/hr	$461,191
Make-up catalyst (Decomposer)		260	$/hr	$1,807,460
ZnO		180	$/hr	$1,252,767
Mol Sieve		81	$/hr	$566,280
Hydrogenation catalyst		20	$/hr	$135,559
Make-up Acid	0.00	115	$/ton	$0.00000
Caustic (ton)	12994	385	$/ton	$4,223,408
Utilities				
Cooling Water	741,688,877	0.005	$/m^3	$3,441,988
Process Water				
Natural	401,419	0.072	$/m^3	$29,086
Softening	1015361	0.065	$/m^3	$65,827
RO/EDI	804859	0.066	$/m^3	$53,353
Process Steam	3468329	0.077	$/kg	$268,535
Electricity	1364605	75	$/Mwe-h	$102,345,358
Heat	2626773.6	30	$/MWt-h	$78,803,208
			TOTAL VARIABLE COSTS	**$204,054,806**
FIXED COSTS				
Maintenance and Repair				$25,524,404
Operating labour + Over head = (20% of labour)				
	Operation - 4 per shift x 4shifts	60	$/hr	$350,400
	Maintenance - 2 per shift x 4 shifts + 6 day shift only	60	$/hr	$149,760
	1 Supervision per shift + 1 maintenance supervision	60	$/hr	$43,800
Insurance	1% of fixed capital			$5,104,881
			TOTAL FIXED COSTS	**$31,173,245**
			TOTAL PRODUCTION COSTS	**$235,228,051**

5.5 Hydrogen Price Component Summary

The cost of hydrogen production by means of the proposed HyS cycles at the various operating conditions is tabulated in Table 24. The table provides a cost component breakdown for each variable case. The breakdown consists of the capital charge, fixed operating and maintenance costs, variable costs and the byproduct credit. The table provides a description of the weight percentage as well as the equivalent cost component that each contributes to the total price per unit. The calculations are based on the results from Table 20-23. Of all the operating conditions the total capital charge and the nuclear heat charge are the two factors that have the most significant impact on the hydrogen production costs, together being responsible for more than 60% of the total production cost.

Table 24: Hydrogen Production Cost Component Summary.

	Case 1 ($/kg)	Weight (%)	Case 2 ($/kg)	Weight (%)	Case 3 ($/kg)	Weight (%)	Case 4 ($/kg)	Weight (%)
Total Capital Charge	**1,44**	**26**	**1,63**	**24**	**1,76**	**23**	**1,60**	**24**
Overnight capital	1,21	22	1,38	20	1,48	19	1,35	21
Replacement capital	0,22	4	0,26	4	0,28	4	0,25	4
Total Fixed O&M:	**0,67**	**12**	**0,76**	**11**	**0,82**	**11**	**0,74**	**11**
Annual Labour	0,01	0	0,01	0	0,02	0	0,01	0
Insurance	0,11	2	0,12	2	0,13	2	0,12	2
Maint. And Repairs	0,55	10	0,62	9	0,67	9	0,60	9
Total Variable O&M:	**3,67**	**68**	**4,68**	**70**	**5,43**	**71**	**4,57**	**70**
Catalyst, Chemicals, Filters	0,17	3	0,19	3	0,21	3	0,19	3
Electricity consumed	2,09	38	2,46	36	2,83	37	2,42	37
Nuclear Heat	1,35	25	1,93	29	2,26	29	1,87	28
Water consumed	0,07	1	0,10	2	0,13	2	0,09	1
Byproduct Credit (O2)	**-0,34**	**-6**	**-0,34**	**-5**	**-0,34**	**-4**	**-0,34**	**-5**
Total Hydrogen Cost ($/kg)	5,44	100	6,73	100	7,67	100	6,57	100

The total hydrogen production cost for Case 1 equals to $5.44/kg. The major contributors are the capital charge (26%), nuclear heat (25%) and electricity consumed (38%).

For Case 2 operating conditions at 40 bar, the total hydrogen production cost is $6.73/kg. The nuclear heat contributes to 29% of the total, followed by the overnight capital (20%) and the electricity consumed (36%).

Case 3 operates at the highest pressure point of 90 bar and produces hydrogen at $7.67/kg. The major contributors are the CAPEX at 19% of the total, nuclear heat at 29% and electricity consumed at 37%.

The total hydrogen costs for Case 4 that operates at a reactor temperature of 750℃ equals to $6.57/kg. The electrical consumption is the prime contributing factor to the total product prices 37%, followed by the CAPEX (21%) and the nuclear heat (28%).

From the hydrogen component price summary the influence of operating temperatures and pressures are clearly reflected in the product price. The results can be applied to determine an optimum operating condition range.

5.6 Sensitivity Analysis

The sensitivity analysis illustrates the effect that certain factors have on the hydrogen price. The sensitivity analysis as performed to determine the factors influencing the hydrogen price namely, the HyS capital, nuclear heat costs, electric consumption (related to process thermal efficiency) and other manufacturing costs. Sensitivity analyses were done for each operating case and are presented in the figures below. The resulting figures indicate which factors the hydrogen production costs are most sensitive to.

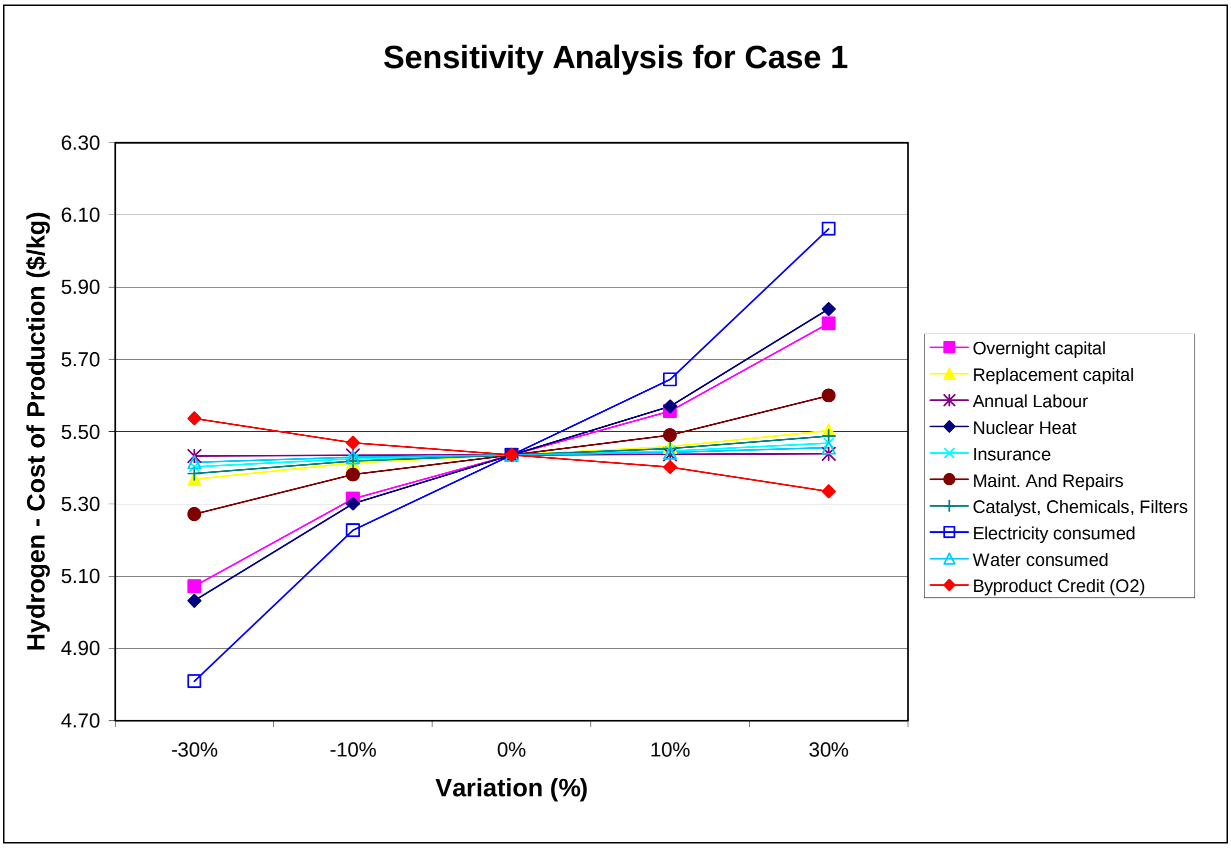

Figure 15: Sensitivity Analysis for Case 1.

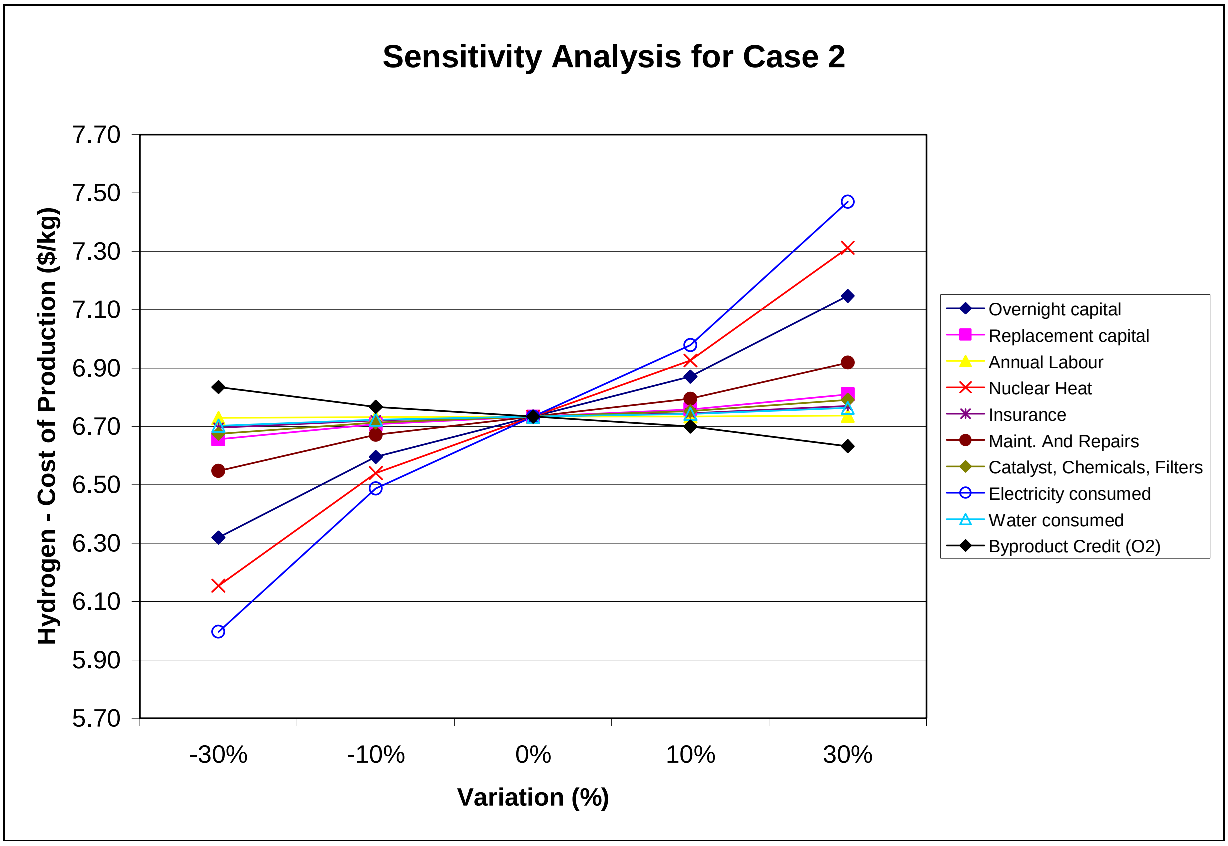

Figure 16: Sensitivity Analysis for Case 2.

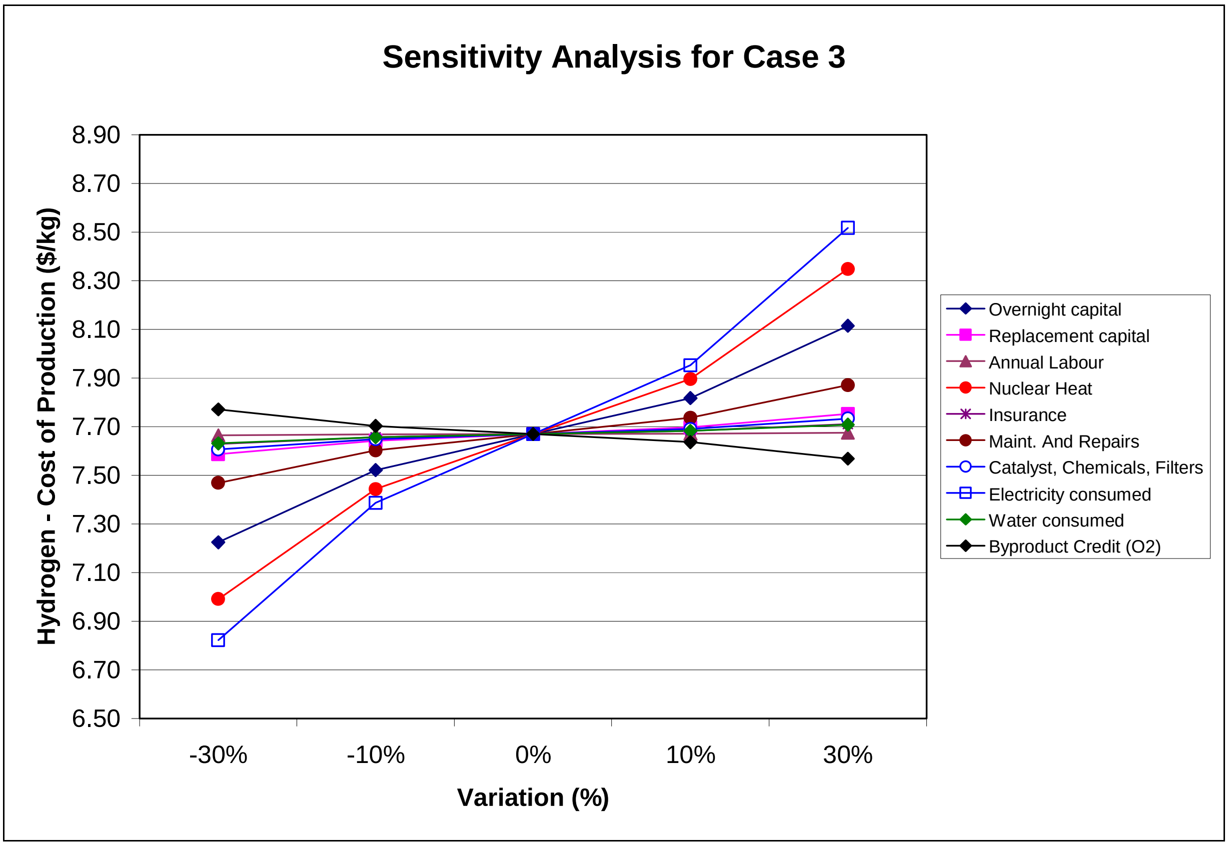

Figure 17: Sensitivity Analysis for Case 3.

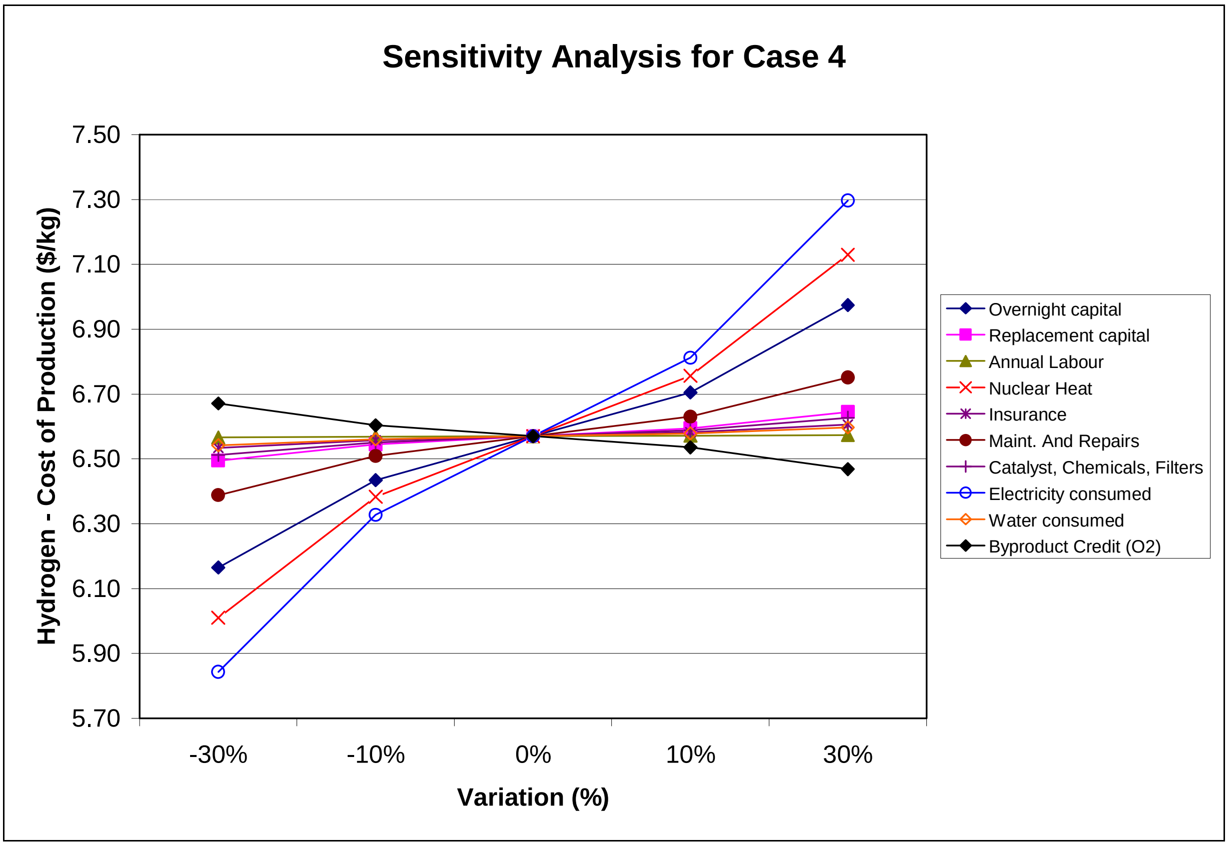

Figure 18: Sensitivity Analysis for Case 4.

From the sensitivity analyses it can be concluded that, for all the cases, the hydrogen production cost is highly sensitive to factors such as the electricity consumption, nuclear heat costs and the required overnight capital of the HyS.

As is evident from the calculation of various hydrogen production cost components (see Table 24), those components that contribute the most to the hydrogen price were electricity costs, nuclear costs and capital costs which is echoed by the sensitivity analysis. The electricity consumed can also be related to the thermal efficiency of the cycle. A higher efficiency will result in a lower electricity import or even result in an electricity export. This effect will benefit the hydrogen production cost positively and will result in a lower hydrogen production cost. The use of thermal heat can be applied more effectively in order to achieve a lower hydrogen production cost. For the capital cost an optimization study could help in lowering the required capital costs and thus lower the sensitivity of the hydrogen production cost to capital cost.

Other factors that were also investigated include variable and fixed costs. These factors seem not to be factors in hydrogen production cost sensitivity and therefore do not require a high level of optimization in order to lower the sensitivity factor.

CHAPTER 6

CONCLUSION AND RECOMMENDATIONS

6. Conclusion and Recommendations

6.1 Conclusion of the Research Project

The global energy sector is experiencing a significant increase in energy demand whilst the non-renewable energy sources are swiftly being depleted. This research project has therefore initiated an investigation into developing a means to address the demand whilst also developing an energy source and carrier that will be clean and environmentally friendly.

A viable source with the most potential of adhering to the criteria is nuclear-produced hydrogen. The method of hydrogen production that is proposed is that of the Hybrid Sulphur Cycle due to its advantages compared to other possible cycles such as the Sulphur-Iodine Cycle or a Steam Methane Reforming process.

The execution of the research project was done by means of Aspen Plus^{TM} as an engineering simulation tool. The models used to achieve accurate results were OLI Mixed Solvent Electrolyte, Oleum Data Package for use with Aspen Plus^{TM}, which provides an accurate representation of the H_2SO_4 properties and ELECNRTL to provide an accurate representation of H_2SO_4 at high temperature conditions.

The technical evaluation of the research project concluded that operating at lower pressures, ranging from 1 - 5 bar, achieves higher overall conversions. The process also favours operating the decomposer reactors at temperatures higher than 750℃, resulting in higher overall conversion and thus higher hydrogen production rates. The results indicate that the advantage of operating at 870℃ and 750℃ can be observed in the higher conversion obtained of SO_3, the increase in the thermal efficiency of the cycle and in the lower cost of production of hydrogen. A higher thermal efficiency is also achieved at lower pressure and higher temperature conditions. The efficiencies that could be obtained, range from 37% - 25% for HHV and 31%-21% for LHV. Higher efficiency can be obtained by optimizing the application of the nuclear heat provided.

A point worth mentioning is that the efficiencies achieved within this study were lower than those achieved in previous studies. This is due to the focus of the study, which was to determine the trend of hydrogen cost ($/kg) with regards to the operating parameters rather than to optimize the process. Factors that play a role in achieving an optimized process are the water balance and the sulphuric acid concentration operating parameters.

Another point of interest is that of the electrolyzer. It was observed that a higher hydrogen production rate results in higher electric requirements of the electrolyzer. Optimization of the design of the electrolyzer system can therefore result in a reduction in electricity consumption with associated operational cost savings. The amount of sulphuric acid within the electrolyzer has an influence on the standard cell voltage, which in turn affects the total cell voltage and electrical requirements of the electrolyzer. The standard cell voltage at 50wt% H_2SO_4 is 0.243V at higher concentration the voltage will increase. However only a slight increase in electrolyzer electrical input is observed.

The production of hydrogen is influenced by the process operating conditions and therefore it also affects the production cost of hydrogen. From the results of the research project it can be concluded that lower operating pressures and higher operating temperatures result in lower hydrogen production costs. The hydrogen production rate is inversely proportional to the function of the capital costs and directly proportional to the function of the electric consumption. An increase in hydrogen production will result in a proportional increase in electrical consumption but only marginal increases in other components to the variable cost. With the current thermal efficiency this results in a lower hydrogen production cost per unit. An increase in hydrogen production will result in a slight increase in the capital cost but will result in a lower hydrogen production cost ($/kg). The electric consumption is a variable cost and comprises approximately 40% of the hydrogen production costs. A method to reduce the electrical consumption must be investigated which could allow the hydrogen costs to become competitive with costs of other means of hydrogen production.

The sensitivity analysis allows the study to identify the factors that need optimization and to identify recommendation for further studies. It can be concluded that the hydrogen cost based on the proposed HyS is sensitive to changes in the capital costs, nuclear heat costs and electrical consumption. The variable costs comprise approximately 70% of the total hydrogen production costs while the fixed costs account for approximately 10% thereof. The capital costs comprise 25% of the total hydrogen production costs.

The oxygen produced as a by-product could be applied as a credit to the hydrogen production costs. This credit lowers the costs by ~5%.

The electrolyzer is the component that contributes to approximately 60% of the electrical consumption of the plant. Since the sensitivity analysis of the plant also indicates that the hydrogen production cost is highly sensitive to the electrical consumption, the efficiency of the electrolyzer should be further investigated. The factors that influence the efficiencies of the electrolyzer are the overpotential, operating temperature of the electrolyzer and the thickness of the electrolyte.

The efficiency of each case study indicates that operating at higher temperatures and lower pressures results in higher efficiencies.

The research project can therefore conclude that the recommended operating parameter range for the HyS to obtain economic viability is at low decomposer operating pressures ranging from 1 - 5 bar and high decomposer operating temperatures at 870℃ or higher.

6.2 Recommendations for Further Studies

The following recommendations are made with regard to a follow-up study:

- An optimization study of the process layout would assist in lowering the capital expenditure required for the proposed HyS cycle, in an attempt to lower the sensitivity of the hydrogen cost on the capital expenditure cost.
- An investigation into achieving an optimal thermal efficiency of the proposed HyS. This can be done by determining the optimal flow path of hot helium generated by a HTGR. An optimal thermal efficiency will result in an optimal electrical consumption. This will affect the hydrogen cost positively and result in more viable energy carrier costs.
- Developing detailed equipment costs specifically for the proposed HyS cycle and the decomposition reactor. This will allow further accuracy in determining the hydrogen production cost.
- An efficiency optimization of the electrolyzer is proposed for further studies. The investigation can include factors such as the thickness of the electrolyte, the operating temperature of the electrolyzer and the overpotential of electrolyzers.

7. References

BALAT, M. 2008. Potential importance of hydrogen as a future solution to environmental and transportation problems. Volume 33, pp 4013-4029.

BOLTHRUNIS, C. 2009. NGNP Hydrogen plant alternatives study. Westinghouse Electric Company LLC, March.

BREY, L, WOITE, G. 1999. Hydrogen as an energy carrier and its production by nuclear power. International Atomic Energy Agency. IAEA-TECDOC--1085.

CHE. 2009. Chemical Engineering. Available from: www.che.com/pci. Date accessed: 2009/11/09

DOUGLAS, J.M. 1988. Conceptual design of chemical processes. MacGraw-Hill. pp 3-95.

FORSBERG, C.W. 2004. Production of hydrogen using nuclear energy. International Scientific Journal for Alternative Energy and Ecology, 2004, **2**, pp 5–9

GORENSEK, M.B. & SUMMERS, W.A. 2008. Hybrid sulphur flowsheets using PEM electrolysis and a bayonet decomposition reactor. International Journal of Hydrogen Energy, 2008, doi: 10.1016/j.ijhydene. 2008.06.049.

GORENSEK, M.B., SUMMERS, W.A., BOLTHRUNIS, C.O., LAHODA, E.J., ALLEN, D.T. & GREYVENSTEIN, R. 2009. Hybrid sulphur process references design and cost analysis. Savannah River National Laboratory, June.

IEO. 2008. International Energy Outlook. The Energy Information Administration of the Department of Energy. Available from: www.eia.doe.gov. Date accessed: 2009/01/19.

JEONG,Y.H., KAZIMI, M.S., HOHNHOLT, K.J & YILDIZ, B. 2005. Optimization of the hybrid sulphur cycle for hydrogen generation,. Nuclear energy and sustainability (NES) program, MIT–NES–TR–004.

LAHODE, E.J., McLAUGHLIN, D.F., MULIK, R., KRIEL, W., KUHR, R., BOLTHRUNIS, C. & CORBETT, M. 2006. Estimated costs for the improved hybrid sulfur (HyS) flowsheet. Westinghouse Science and Technology Department, Shaw Stone and Webster.

McHUGH, K., EISELE, S. & NESTELL, J. 2005. Hydrogen production methods. MRP Associates Inc., MPR-WP-0001, February.

MIDILLI, A. & DINCER, I. 2008. Hydrogen as a renewable and sustainable solution in reducing global fossil fuel consumption. International journal of hydrogen energy. Volume 33, pp 4209-4222.

NI, M., LEUNG, M. & LEUNG, D. 2008. Energy and exergy analysis of hydrogen production by a proton exchange membrane (PEM) electrolyzer plant. Energy Conversion and Management, Volume 49, pp 2748-2756.

PETERS, M.S., TIMMERHAUS, K.O. & WEST, R.E. 2003. Plant design and economics for chemical engineers. McGraw-Hill, Fifth Edition, 2003. pp 230-278.

SUMMERS, W.A., GORENSEK, M.B. & BUCKNER, M.R. YEAR. The hybrid sulphur cycle for nuclear hydrogen production. Savannah River National Laboratory, WSRC-MS-2005-00509.

ULRICH, G.D. & VASUDEVAN, P.T. 2006. How to estimate utility costs. University of New Hampshire, Chemical Engineering, April.

WEO. 2008. World Energy Outlook. The Energy Information Administration of the International Energy Agency. Available from: www.worldenergyoutlook.org . Date accessed: 2009/01/19.

YILDIZ, B., PETRI, M.C., CONZELMANN, G. & FORSBERG, C. 2005. Configuration and technology implications of potential nuclear hydrogen system applications. Argonne National Laboratory. July.

ZERTA, M., SCHMIDT, P.R., STILLER, C. & LANDINGER, H. 2008. Alternative world energy outlook (AWEO) and the role of the hydrogen in a changing energy landscape. International journal of hydrogen energy. Volume 33, pp 3021-3025.

8. Appendix A: HyS flowsheets

Case 1

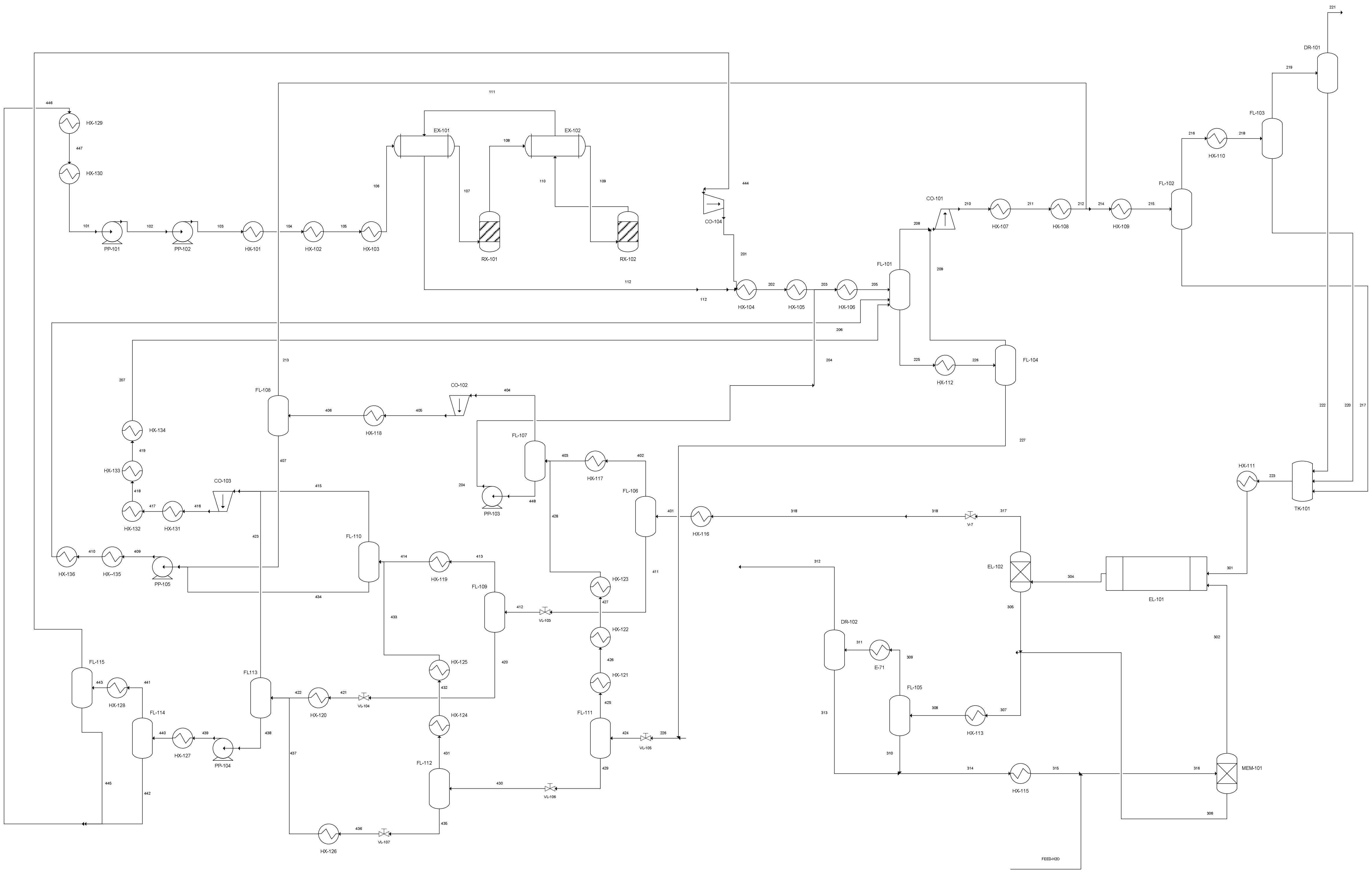

Figure 19: HyS flowsheet Case 1

Case 2

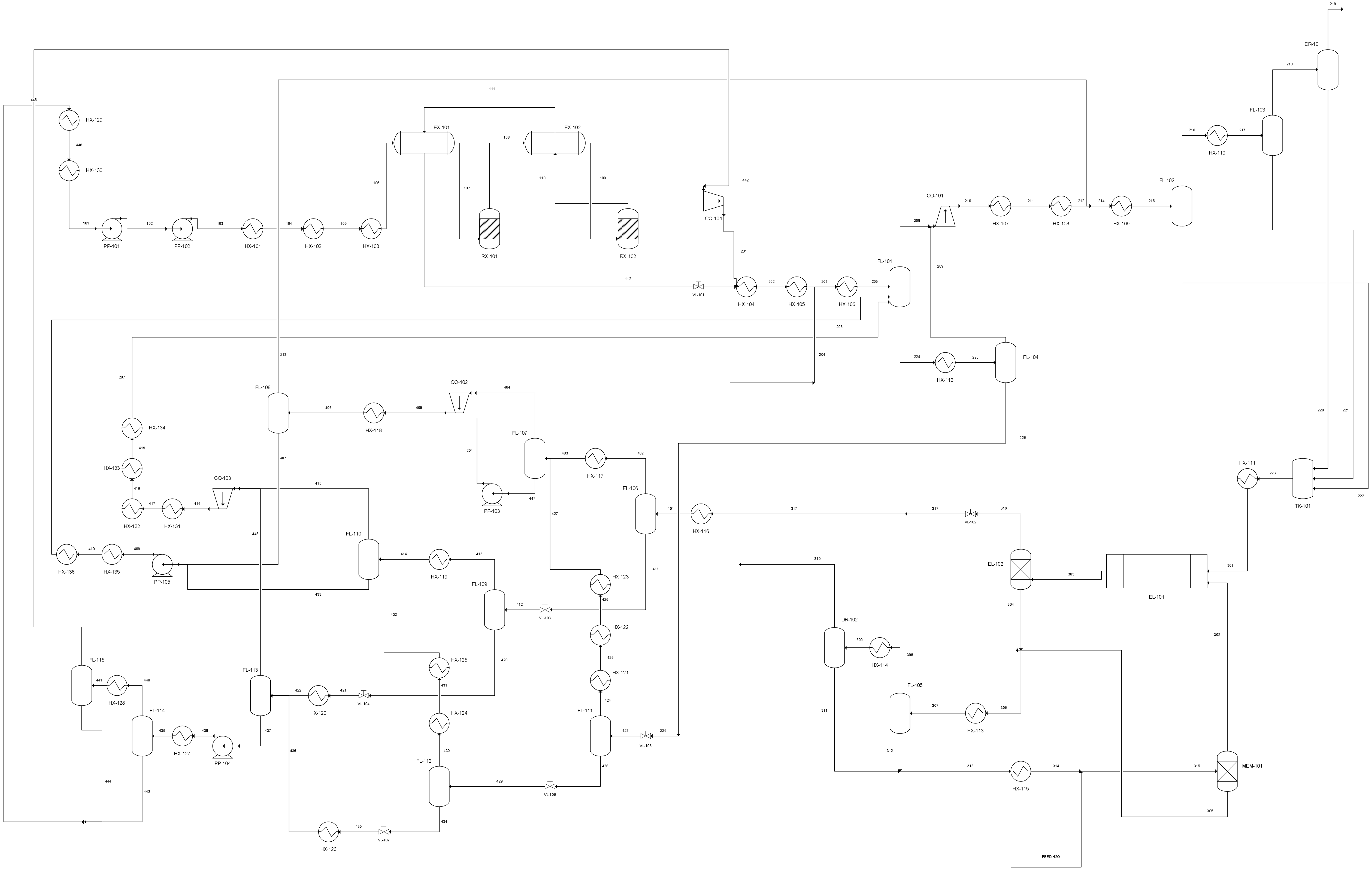

Figure 20: HyS flowsheet Case 2

Case 3

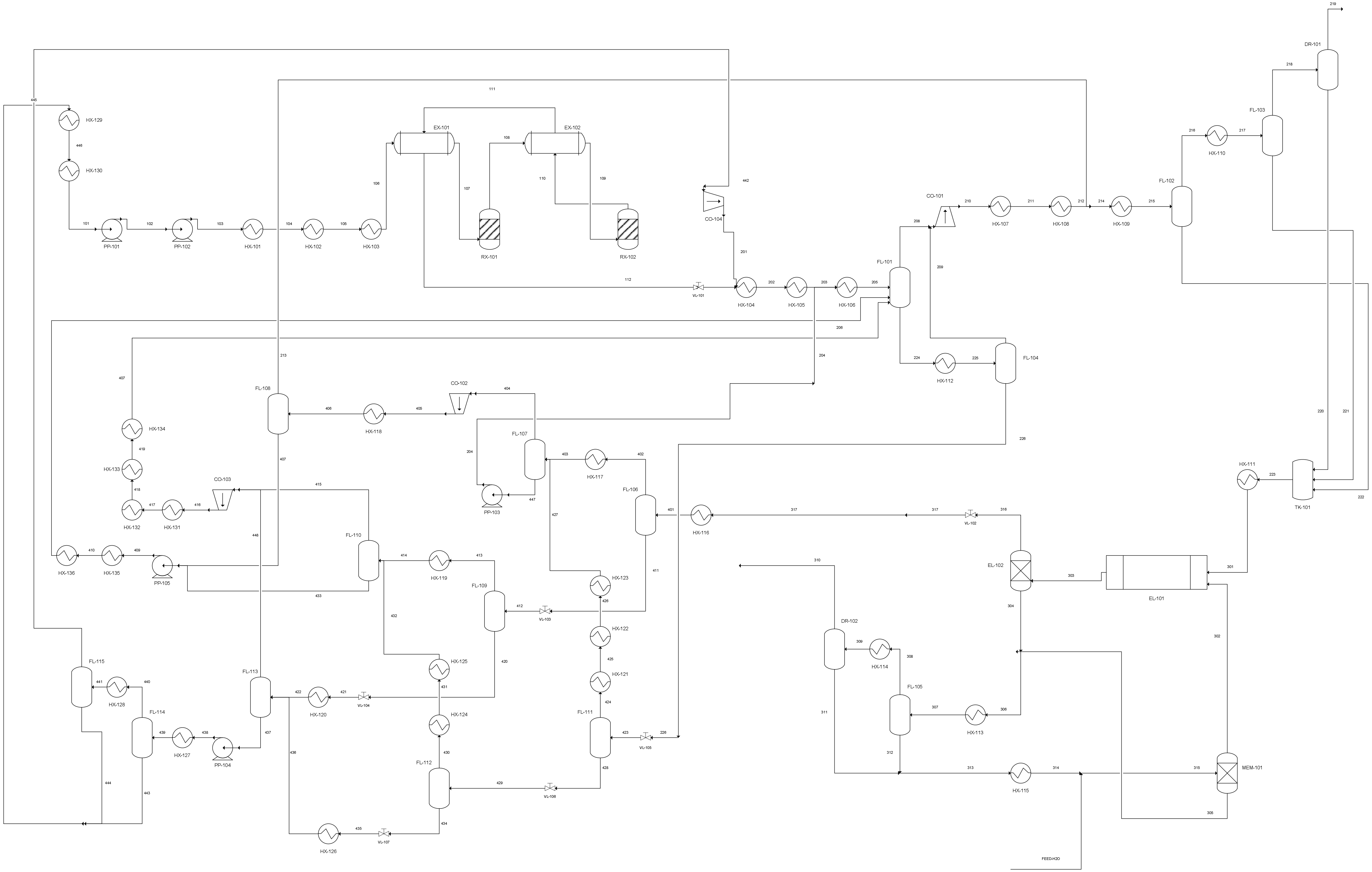

Figure 21: HyS flowsheet Case 3

Case 4

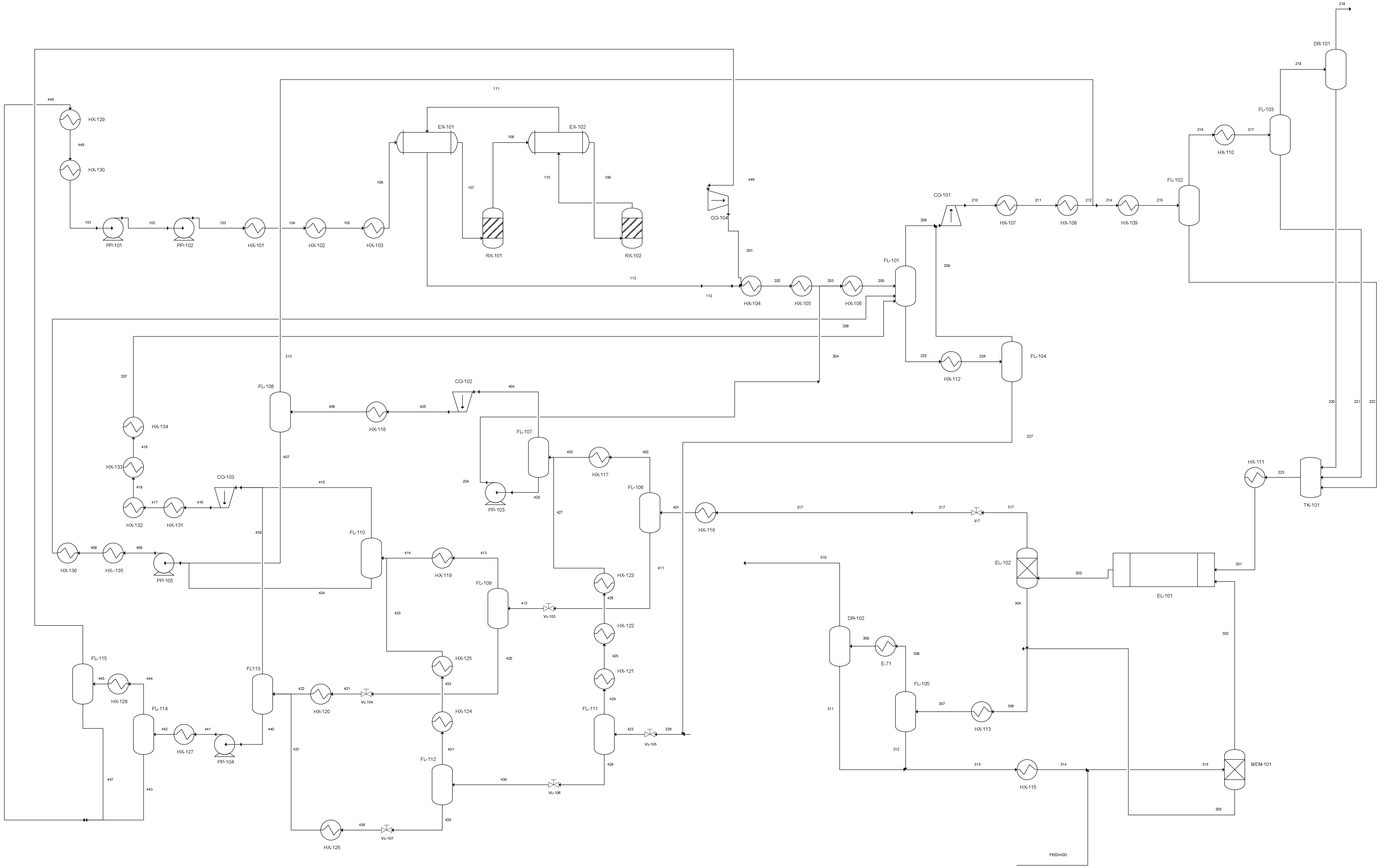

Figure 22: HyS flowsheet Case 4

9. Appendix B: Mass Balance

Mass Balance: Case 1

Table 25: Mass Balance for Case 1

	101	102	103	104	105	106	107	108	109	110
To	PP-101	PP-102	HX-101	HX-102	HX-103	EX-101	RX-101	EX-102	RX-102	EX-102
From		PP-101	PP-102	HX-101	HX-102	HX-103	EX-101	RX-101	EX-102	RX-102
	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	VAPOR	VAPOR	VAPOR	VAPOR	VAPOR
Substream: MIXED										
Mole Flow kmol/sec										
H2O	0.20	0.20	0.20	0.29	0.31	1.08	1.39	1.67	1.68	1.68
H2SO4	1.21	1.21	1.21	1.30	1.33	0.61	0.30	0.02	0.01	0.00
H2	-	-	-	-	-	-	-	-	-	-
O2	-	-	-	-	-	-	-	-	-	0.48
SO2	-	-	-	-	-	-	-	-	-	0.97
SO3	0.00	0.00	0.00	0.00	0.00	0.74	1.05	1.33	1.34	0.38
OH-	0.00	0.00	0.00	0.00	0.00	-	-	-	-	-
HSO3-	-	-	-	-	-	-	-	-	-	-
HSO4-	0.14	0.14	0.14	0.05	0.02	-	-	-	-	-
H3O+	0.14	0.14	0.14	0.05	0.02	-	-	-	-	-
SO3-2	-	-	-	-	-	-	-	-	-	-
SO4-2	0.00	0.00	0.00	0.00	0.00	-	-	-	-	-
Mass Flow kg/sec										
H2O	3.62	3.62	3.62	5.23	5.65	19.48	24.97	30.07	30.31	30.31
H2SO4	119.00	119.00	119.00	127.73	129.96	59.46	29.56	1.77	0.49	0.49
H2	-	-	-	-	-	-	-	-	-	-
O2	-	-	-	-	-	-	-	-	-	15.49
SO2	-	-	-	-	-	-	-	-	-	62.04
SO3	0.00	0.00	0.00	0.03	0.05	59.55	83.96	106.64	107.69	30.15
OH-	0.00	0.00	0.00	0.00	0.00	-	-	-	-	-
HSO3-	-	-	-	-	-	-	-	-	-	-
HSO4-	13.27	13.27	13.27	4.60	2.36	-	-	-	-	-
H3O+	2.60	2.60	2.60	0.90	0.46	-	-	-	-	-
SO3-2	-	-	-	-	-	-	-	-	-	-
SO4-2	0.00	0.00	0.00	0.00	0.00	-	-	-	-	-
Total Flow kmol/sec	1.69	1.69	1.69	1.69	1.69	2.43	2.74	3.02	3.03	3.52
Total Flow kg/sec	138.49	138.49	138.49	138.49	138.49	138.49	138.49	138.49	138.49	138.48
Total Flow cum/sec	0.08	0.08	0.08	0.09	0.09	43.40	52.87	68.79	83.96	111.45
Temperature K	439.00	439.02	439.09	579.00	610.00	651.30	700.68	823.15	999.24	1,143.15
Pressure bar	1.00	1.50	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00
Vapor Frac	-	-	-	-	-	1.00	1.00	1.00	1.00	1.00
Liquid Frac	1.00	1.00	1.00	1.00	1.00	-	-	-	-	-

Table 26: Mass Balance for Case 1

	111	112	201	202	203	204	205	206	207	208
To	EX-101	HX-104	HX-104	HX-105	HX-106	HX-106	FL-101	FL-101	FL-101	CO-101
From	EX-102	EX-101	CO-104	HX-104	HX-105	PP-103	HX-106	HX-136	HX-134	FL-101
	VAPOR	VAPOR	VAPOR	MIXED	MIXED	LIQUID	MIXED	MIXED	MIXED	VAPOR
Substream: MIXED										
Mole Flow kmol/sec										
H2O	1.69	1.66	0.92	2.33	2.17	0.00	1.69	0.09	0.00	0.39
H2SO4	0.00	0.03	0.10	0.37	0.45	0.00	0.01	0.00	0.00	0.00
H2	-	-	-	-	-	-	-	-	-	-
O2	0.48	0.48	0.00	0.48	0.48	0.00	0.48	0.00	0.00	0.48
SO2	0.97	0.97	0.00	0.97	0.97	0.00	0.97	0.00	0.01	0.97
SO3	0.38	0.35	0.02	0.13	0.01	0.00	0.00	0.00	0.00	0.00
OH-	-	-	-	0.00	0.00	0.00	0.00	0.00	0.00	-
HSO3-	-	-	-	0.00	0.00	0.00	0.00	0.00	0.00	-
HSO4-	-	-	-	0.00	0.04	0.00	0.47	0.00	0.00	-
H3O+	-	-	-	0.00	0.04	0.00	0.52	0.00	0.00	-
SO3-2	-	-	-	-	0.00	0.00	0.00	0.00	0.00	-
SO4-2	-	-	-	0.00	0.00	0.00	0.02	0.00	0.00	-
Mass Flow kg/sec										
H2O	30.37	29.87	16.53	41.99	39.08	0.00	30.40	1.57	0.02	6.97
H2SO4	0.18	2.91	9.59	36.51	44.00	0.00	0.74	0.00	0.00	0.00
H2	-	-	-	-	-	-	-	-	-	-
O2	15.49	15.49	0.00	15.49	15.49	0.00	15.49	0.00	0.00	15.49
SO2	62.04	62.04	0.08	62.12	62.12	0.00	62.12	0.14	0.50	62.20
SO3	30.40	28.18	1.66	10.23	0.71	0.00	0.00	0.00	0.00	0.00
OH-	-	-	-	0.00	0.00	0.00	0.00	0.00	0.00	-
HSO3-	-	-	-	0.00	0.00	0.00	0.00	0.00	0.00	-
HSO4-	-	-	-	0.00	4.13	0.00	45.59	0.00	0.00	-
H3O+	-	-	-	0.00	0.81	0.00	9.81	0.00	0.00	-
SO3-2	-	-	-	-	0.00	0.00	0.00	0.00	0.00	-
SO4-2	-	-	-	0.00	0.00	0.00	2.20	0.00	0.00	-
Total Flow kmol/sec	3.52	3.49	1.04	4.28	4.17	0.00	4.16	0.09	0.01	1.84
Total Flow kg/sec	138.48	138.48	27.86	166.34	166.34	0.00	166.35	1.71	0.52	84.67
Total Flow cum/sec	93.65	73.37	21.56	71.96	56.71	0.00	19.49	0.06	0.09	19.81
Temperature K	960.00	759.00	752.73	613.15	573.15	343.15	393.15	393.00	393.00	393.15
Pressure bar	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00
Vapor Frac	1.00	1.00	1.00	0.99	0.86	-	0.43	0.07	1.00	1.00
Liquid Frac	-	-	-	0.01	0.14	1.00	0.57	0.93	0.00	-

Table 27: Mass Balance for Case 1

	209	210	211	212	213	214	215	216	217	218
To	CO-101	HX-107	HX-108	MX-101	MX-101	HX-109	FL-102	HX-110	TK-101	FL-103
From	FL-104	CO-101	HX-107	HX-108	FL-108	MX-101	HX-109	FL-102	FL-102	HX-110
	VAPOR	VAPOR	VAPOR	MIXED	VAPOR	MIXED	MIXED	VAPOR	LIQUID	MIXED
Substream: MIXED										
Mole Flow kmol/sec										
H2O	1.10	1.48	1.48	1.48	0.06	1.54	1.46	0.00	1.45	0.00
H2SO4	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-
H2	-	-	-	-	-	-	-	-	-	-
O2	0.00	0.48	0.48	0.48	0.00	0.49	0.49	0.48	0.00	0.48
SO2	0.01	0.98	0.98	0.98	0.97	1.95	1.91	0.23	1.67	0.23
SO3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-
OH-	-	-	-	0.00	-	0.00	0.00	-	0.00	0.00
HSO3-	-	-	-	0.00	-	0.00	0.04	-	0.04	0.00
HSO4-	-	-	-	0.00	-	0.00	0.00	-	0.00	-
H3O+	-	-	-	0.00	-	0.00	0.04	-	0.04	0.00
SO3-2	-	-	-	0.00	-	0.00	0.00	-	0.00	0.00
SO4-2	-	-	-	0.00	-	0.00	0.00	-	0.00	-
Mass Flow kg/sec										
H2O	19.77	26.74	26.74	26.73	1.08	27.81	26.23	0.07	26.16	0.03
H2SO4	0.04	0.04	0.04	0.00	0.00	0.00	0.00	0.00	0.00	-
H2	-	-	-	-	-	-	-	-	-	-
O2	0.00	15.49	15.49	15.49	0.08	15.57	15.57	15.51	0.06	15.51
SO2	0.56	62.76	62.76	62.76	62.35	125.11	122.31	15.03	107.27	14.98
SO3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-
OH-	-	-	-	0.00	-	0.00	0.00	-	0.00	0.00
HSO3-	-	-	-	0.00	-	0.00	3.54	-	3.55	0.07
HSO4-	-	-	-	0.04	-	0.04	0.00	-	0.00	-
H3O+	-	-	-	0.01	-	0.01	0.85	-	0.85	0.02
SO3-2	-	-	-	0.00	-	0.00	0.00	-	0.00	0.00
SO4-2	-	-	-	0.00	-	0.00	0.04	-	0.04	-
Total Flow kmol/sec	1.11	2.95	2.95	2.95	1.04	3.98	3.94	0.72	3.22	0.72
Total Flow kg/sec	20.36	105.03	105.03	105.03	63.51	168.54	168.54	30.61	137.93	30.61
Total Flow cum/sec	15.33	8.56	6.83	5.51	1.26	6.75	0.94	0.84	0.09	0.49
Temperature K	506.00	739.67	600.00	500.00	373.00	463.13	313.15	313.00	313.00	250.00
Pressure bar	3.00	21.00	21.00	21.00	21.00	21.00	21.00	21.00	21.00	21.00
Vapor Frac	1.00	1.00	1.00	1.00	1.00	1.00	0.18	1.00	-	0.70
Liquid Frac	-	-	-	0.00	-	0.00	0.82	-	1.00	0.30

Table 28: Mass Balance for Case 1

	219	220	221	222	223	224	225	226	301	302
To	DR-101	TK-101		TK-101	HX-111	HX-112	FL-104	VL-104	EL-101	EL-101
From	FL-103	FL-103	DR-101	DR-101	TK-101	FL-101	HX-112	FL-104	HX-111	MEM-101
	VAPOR	LIQUID	VAPOR	LIQUID	MIXED	LIQUID	MIXED	LIQUID	LIQUID	LIQUID
Substream: MIXED										
Mole Flow kmol/sec										
H2O	0.00	0.00	-	0.00	1.44	1.39	1.57	0.47	1.51	0.96
H2SO4	-	-	-	-	0.00	0.01	0.17	0.17	0.00	0.00
H2	-	-	-	-	-	-	-	-	-	0.00
O2	0.48	0.00	0.48	-	0.00	0.00	0.00	0.00	0.00	-
SO2	0.02	0.21	-	0.02	1.90	0.01	0.01	0.00	1.94	-
SO3	-	-	-	-	0.00	0.00	0.00	0.00	0.00	0.00
OH-	-	0.00	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HSO3-	-	0.00	-	0.00	0.05	0.00	0.00	0.00	0.02	-
HSO4-	-	-	-	-	0.00	0.47	0.33	0.33	0.00	0.00
H3O+	-	0.00	-	0.00	0.05	0.52	0.33	0.33	0.02	0.00
SO3-2	-	0.00	-	0.00	0.00	0.00	0.00	0.00	0.00	-
SO4-2	-	-	-	-	0.00	0.02	0.00	0.00	0.00	0.00
Mass Flow kg/sec										
H2O	0.00	0.03	-	0.00	25.99	24.98	28.32	8.55	27.23	17.38
H2SO4	-	-	-	-	0.00	0.68	16.50	16.46	0.00	0.00
H2	-	-	-	-	-	-	-	-	-	0.00
O2	15.49	0.01	15.49	-	0.08	0.00	0.00	0.00	0.08	-
SO2	1.36	13.61	-	1.36	121.89	0.56	0.56	0.00	124.08	-
SO3	-	-	-	-	0.00	0.00	0.00	0.00	0.00	0.00
OH-	-	0.00	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HSO3-	-	0.07	-	0.00	4.08	0.00	0.00	0.00	1.30	-
HSO4-	-	-	-	-	0.00	45.56	32.21	32.21	0.02	0.01
H3O+	-	0.02	-	0.00	0.97	9.84	6.31	6.31	0.32	0.00
SO3-2	-	0.00	-	0.00	0.00	0.00	0.00	0.00	0.00	-
SO4-2	-	-	-	-	0.04	2.29	0.00	0.00	0.02	0.00
Total Flow kmol/sec	0.51	0.22	0.48	0.02	3.45	2.41	2.41	1.31	3.48	0.97
Total Flow kg/sec	16.86	13.75	15.49	1.36	153.04	83.91	83.91	63.54	153.04	17.39
Total Flow cum/sec	0.48	0.01	0.47	0.00	0.10	0.06	15.38	0.05	0.11	0.02
Temperature K	250.00	250.00	250.00	250.00	309.45	393.15	506.00	506.00	373.15	373.08
Pressure bar	21.00	21.00	21.00	21.00	21.00	3.00	3.00	3.00	21.00	21.00
Vapor Frac	1.00	-	1.00	-	0.00	-	0.46	-	-	-
Liquid Frac	-	1.00	-	1.00	1.00	1.00	0.54	1.00	1.00	1.00

Table 29: Mass Balance for Case 1

	304	305	306	307	308	309	310	311	312	313
To	EL-102	MX-102	MX-102	HX-113	FL-105	HX-114	MX-103	DR-102		MX-103
From	EL-101	EL-102	MEM-101	MX-102	HX-113	FL-105	FL-105	HX-114	DR-102	DR-102
	MIXED	VAPOR	LIQUID	MIXED	MIXED	VAPOR	LIQUID	MIXED	VAPOR	LIQUID
Substream: MIXED										
Mole Flow kmol/sec										
H2O	0.20	-	0.97	0.97	0.97	0.02	0.95	0.02	-	0.02
H2SO4	0.60	-	-	-	-	-	-	-	-	-
H2	0.97	0.97	-	0.97	0.97	0.97	0.00	0.97	0.97	-
O2	0.00	-	-	-	-	-	-	-	-	-
SO2	0.98	-	-	-	-	-	-	-	-	-
SO3	0.00	-	-	-	-	-	-	-	-	-
OH-	0.00	-	0.00	0.00	0.00	-	0.00	0.00	-	0.00
HSO3-	0.00	-	-	-	-	-	-	-	-	-
HSO4-	0.37	-	-	-	-	-	-	-	-	-
H3O+	0.37	-	0.00	0.00	0.00	-	0.00	0.00	-	0.00
SO3-2	0.00	-	-	-	-	-	-	-	-	-
SO4-2	0.00	-	-	-	-	-	-	-	-	-
Mass Flow kg/sec										
H2O	3.57	-	17.39	17.39	17.39	0.33	17.05	0.33	-	0.33
H2SO4	58.40	-	-	-	-	-	-	-	-	-
H2	1.95	1.95	-	1.95	1.95	1.95	0.00	1.95	1.95	-
O2	0.08	-	-	-	-	-	-	-	-	-
SO2	63.07	-	-	-	-	-	-	-	-	-
SO3	0.00	-	-	-	-	-	-	-	-	-
OH-	0.00	-	0.00	0.00	0.00	-	0.00	0.00	-	0.00
HSO3-	0.00	-	-	-	-	-	-	-	-	-
HSO4-	36.17	-	-	-	-	-	-	-	-	-
H3O+	7.12	-	0.00	0.00	0.00	-	0.00	0.00	-	0.00
SO3-2	0.00	-	-	-	-	-	-	-	-	-
SO4-2	0.08	-	-	-	-	-	-	-	-	-
Total Flow kmol/sec	3.50	0.97	0.97	1.93	1.93	0.99	0.95	0.99	0.97	0.02
Total Flow kg/sec	170.44	1.95	17.39	19.34	19.34	2.29	17.05	2.29	1.95	0.33
Total Flow cum/sec	2.74	1.45	0.02	1.46	1.40	1.38	0.02	1.28	1.28	0.00
Temperature K	373.15	373.15	373.08	360.55	348.15	348.15	348.15	313.15	313.15	313.15
Pressure bar	21.00	21.00	21.00	21.00	21.00	21.00	21.00	20.00	20.00	20.00
Vapor Frac	0.53	1.00	-	0.52	0.51	1.00	-	0.98	1.00	-
Liquid Frac	0.47	-	1.00	0.48	0.49	-	1.00	0.02	-	1.00

Table 30: Mass Balance for Case 1

	314	315	316	317	318	401	402	403	404	405
To	HX-115	MX-104	MEM-101	VL-101	HX-116	FL-106	HX-117	FL-107	CO-102	HX-118
From	MX-103	HX-115	MX-104	EL-102	VL-101	HX-116	FL-106	HX-117	FL-107	CO-102
	MIXED	LIQUID	LIQUID	MIXED	MIXED	MIXED	VAPOR	MIXED	VAPOR	VAPOR
Substream: MIXED										
Mole Flow kmol/sec										
H2O	0.97	0.97	1.93	0.10	0.10	0.21	0.00	0.00	0.08	0.08
H2SO4	-	-	0.00	0.51	0.50	0.61	0.00	0.00	0.00	0.00
H2	0.00	0.00	0.00	-	-	-	-	-	-	-
O2	-	-	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO2	-	-	-	0.98	0.98	0.98	0.98	0.98	0.98	0.98
SO3	-	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00	-	-
HSO3-	-	-	-	0.00	0.00	0.00	-	0.00	-	-
HSO4-	-	-	0.00	0.45	0.47	0.36	-	0.00	-	-
H3O+	0.00	0.00	0.00	0.47	0.47	0.36	-	0.00	-	-
SO3-2	-	-	-	0.00	0.00	0.00	-	0.00	-	-
SO4-2	-	-	0.00	0.01	0.00	0.00	-	0.00	-	-
Mass Flow kg/sec										
H2O	17.39	17.39	34.77	1.86	1.80	3.75	0.03	0.03	1.41	1.41
H2SO4	-	-	0.00	49.89	48.79	59.40	0.00	0.00	0.00	0.00
H2	0.00	0.00	0.00	-	-	-	-	-	-	-
O2	-	-	-	0.08	0.08	0.08	0.08	0.08	0.08	0.08
SO2	-	-	-	63.07	63.07	63.07	62.48	62.48	62.48	62.48
SO3	-	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00	-	-
HSO3-	-	-	-	0.00	0.00	0.00	-	0.00	-	-
HSO4-	-	-	0.01	43.88	45.74	35.22	-	0.00	-	-
H3O+	0.00	0.00	0.00	8.92	8.98	6.92	-	0.00	-	-
SO3-2	-	-	-	0.00	0.00	0.00	-	0.00	-	-
SO4-2	-	-	0.00	0.80	0.04	0.06	-	0.00	-	-
Total Flow kmol/sec	0.97	0.97	1.93	2.53	2.53	2.53	0.98	0.98	1.06	1.06
Total Flow kg/sec	17.39	17.39	34.78	168.50	168.50	168.50	62.58	62.58	63.97	63.97
Total Flow cum/sec	0.02	0.02	0.04	0.11	20.59	29.56	29.50	27.67	29.83	2.91
Temperature K	347.50	373.00	373.08	373.15	278.45	365.00	365.00	343.00	343.00	702.91
Pressure bar	20.00	21.00	21.00	21.00	1.00	1.00	1.00	1.00	1.00	21.00
Vapor Frac	0.00	-	-	0.00	0.36	0.39	1.00	1.00	1.00	1.00
Liquid Frac	1.00	1.00	1.00	1.00	0.64	0.61	-	0.00	-	-

Table 31: Mass Balance for Case 1

	406	407	408	409	410	411	412	413	414	415
To	FL-108	MX-106	PP-105	HX-135	HX-136	VL-102	FL-109	HX-119	FL-110	CO-103
From	HX-118	FL-108	MX-106	PP-105	HX-135	FL-106	VL-102	FL-109	HX-119	FL-110
	MIXED	LIQUID	MIXED	MIXED	MIXED	LIQUID	MIXED	VAPOR	MIXED	VAPOR
Substream: MIXED										
Mole Flow kmol/sec										
H2O	0.08	0.02	0.09	0.09	0.09	0.21	0.21	0.00	0.00	0.00
H2SO4	0.00	0.00	0.00	0.00	0.00	0.61	0.61	0.00	0.00	0.00
H2	-	-	-	-	-	-	-	-	-	-
O2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO2	0.98	0.00	0.00	0.00	0.00	0.01	0.01	0.00	0.00	0.00
SO3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00	-
HSO3-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00	-
HSO4-	0.00	0.00	0.00	0.00	0.00	0.36	0.36	-	0.00	-
H3O+	0.00	0.00	0.00	0.00	0.00	0.36	0.36	-	0.00	-
SO3-2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00	-
SO4-2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00	-
Mass Flow kg/sec										
H2O	1.41	0.33	1.56	1.56	1.56	3.72	3.73	0.00	0.00	0.01
H2SO4	0.00	0.00	0.00	0.00	0.00	59.40	59.44	0.00	0.00	0.00
H2	-	-	-	-	-	-	-	-	-	-
O2	0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO2	62.48	0.12	0.14	0.13	0.14	0.59	0.59	0.18	0.18	0.16
SO3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00	-
HSO3-	0.00	0.00	0.00	0.01	0.01	0.00	0.00	-	0.00	-
HSO4-	0.00	0.00	0.00	0.00	0.00	35.22	35.19	-	0.00	-
H3O+	0.00	0.00	0.00	0.00	0.00	6.92	6.92	-	0.00	-
SO3-2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00	-
SO4-2	0.00	0.00	0.00	0.00	0.00	0.06	0.05	-	0.00	-
Total Flow kmol/sec	1.06	0.02	0.09	0.09	0.09	1.55	1.55	0.00	0.00	0.00
Total Flow kg/sec	63.97	0.46	1.71	1.71	1.71	105.92	105.92	0.18	0.18	0.17
Total Flow cum/sec	1.27	0.00	0.24	0.01	0.01	0.06	0.72	0.25	0.24	0.29
Temperature K	373.00	373.00	316.23	337.94	350.00	365.00	364.22	325.00	313.00	313.00
Pressure bar	21.00	21.00	0.30	3.00	3.00	1.00	0.30	0.30	0.30	0.30
Vapor Frac	0.98	-	0.03	0.00	0.01	-	0.00	1.00	1.00	1.00
Liquid Frac	0.02	1.00	0.97	1.00	0.99	1.00	1.00	-	0.00	-

Table 32: Mass Balance for Case 1

	416	417	418	419	420	421	422	423	424	425
To	HX-131	HX-132	HX-133	HX-134	VL-103	HX-120	FL-113	CO-103	FL-111	HX-121
From	CO-103	HX-131	HX-132	HX-133	FL-109	VL-103	HX-120	FL-113	VL-104	FL-111
	VAPOR	VAPOR	VAPOR	VAPOR	LIQUID	MIXED	MIXED	VAPOR	MIXED	VAPOR
Substream: MIXED										
Mole Flow kmol/sec										
H2O	0.00	0.00	0.00	0.00	0.16	0.16	0.21	0.00	0.47	0.08
H2SO4	0.00	0.00	0.00	0.00	0.56	0.56	0.61	0.00	0.17	0.00
H2	-	-	-	-	-	-	-	-	-	-
O2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO2	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.00	0.00
SO3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-	-	-	-	-	0.00	0.00	0.00	-	0.00	-
HSO3-	-	-	-	-	0.00	0.00	0.00	-	0.00	-
HSO4-	-	-	-	-	0.41	0.41	0.36	-	0.33	-
H3O+	-	-	-	-	0.41	0.41	0.36	-	0.33	-
SO3-2	-	-	-	-	0.00	0.00	0.00	-	0.00	-
SO4-2	-	-	-	-	0.00	0.00	0.00	-	0.00	-
Mass Flow kg/sec										
H2O	0.02	0.02	0.02	0.02	2.89	2.90	3.85	0.00	8.51	1.39
H2SO4	0.00	0.00	0.00	0.00	54.92	54.96	60.12	0.00	16.24	0.00
H2	-	-	-	-	-	-	-	-	-	-
O2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO2	0.50	0.50	0.50	0.50	0.42	0.42	0.42	0.34	0.00	0.00
SO3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-	-	-	-	-	0.00	0.00	0.00	-	0.00	-
HSO3-	-	-	-	-	0.00	0.00	0.00	-	0.00	-
HSO4-	-	-	-	-	39.64	39.61	34.52	-	32.41	-
H3O+	-	-	-	-	7.80	7.79	6.78	-	6.36	-
SO3-2	-	-	-	-	0.00	0.00	0.00	-	0.00	-
SO4-2	-	-	-	-	0.07	0.07	0.05	-	0.01	-
Total Flow kmol/sec	0.01	0.01	0.01	0.01	1.55	1.55	1.55	0.01	1.31	0.08
Total Flow kg/sec	0.52	0.52	0.52	0.52	105.74	105.74	105.74	0.34	63.54	1.39
Total Flow cum/sec	0.19	0.17	0.16	0.15	0.06	1.23	1.85	1.70	3.33	3.00
Temperature K	767.73	685.00	645.00	600.00	325.00	324.58	370.00	370.00	472.69	472.00
Pressure bar	3.00	3.00	3.00	3.00	0.30	0.10	0.10	0.10	1.00	1.00
Vapor Frac	1.00	1.00	1.00	1.00	-	0.00	0.00	1.00	0.06	1.00
Liquid Frac	-	-	-	-	1.00	1.00	1.00	-	0.94	-

Table 33: Mass Balance for Case 1

	426	427	428	429	430	431	432	433	434	435
To	HX-122	HX-123	FL-107	VL-105	FL-112	HX-124	HX-125	FL-110	MX-106	VL-106
From	HX-121	HX-122	HX-123	FL-111	VL-105	FL-112	HX-124	HX-125	FL-110	FL-112
	MIXED	MIXED	LIQUID	LIQUID	MIXED	VAPOR	MIXED	LIQUID	LIQUID	LIQUID
Substream: MIXED										
Mole Flow kmol/sec										
H2O	0.08	0.08	0.08	0.39	0.39	0.07	0.07	0.07	0.07	0.32
H2SO4	0.00	0.00	0.00	0.16	0.16	0.00	0.00	0.00	0.00	0.16
H2	-	-	-	-	-	-	-	-	-	-
O2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-	0.00	0.00	0.00	0.00	0.00	-	0.00	0.00	0.00	0.00
HSO3-	0.00	0.00	0.00	0.00	0.00	-	0.00	0.00	0.00	0.00
HSO4-	0.00	0.00	0.00	0.34	0.34	-	0.00	0.00	0.00	0.34
H3O+	0.00	0.00	0.00	0.34	0.34	-	0.00	0.00	0.00	0.34
SO3-2	0.00	0.00	0.00	0.00	0.00	-	0.00	0.00	0.00	0.00
SO4-2	0.00	0.00	0.00	0.00	0.00	-	0.00	0.00	0.00	0.00
Mass Flow kg/sec										
H2O	1.38	1.38	1.38	7.07	7.07	1.25	1.25	1.25	1.23	5.76
H2SO4	0.00	0.00	0.00	15.96	15.97	0.00	0.00	0.00	0.00	15.61
H2	-	-	-	-	-	-	-	-	-	-
O2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.01	0.00
SO3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-	0.00	0.00	0.00	0.00	0.00	-	0.00	0.00	0.00	0.00
HSO3-	0.00	0.00	0.00	0.00	0.00	-	0.00	0.00	0.00	0.00
HSO4-	0.00	0.00	0.00	32.69	32.66	-	0.00	0.00	0.00	33.01
H3O+	0.00	0.00	0.00	6.41	6.41	-	0.00	0.00	0.00	6.48
SO3-2	0.00	0.00	0.00	0.00	0.00	-	0.00	0.00	0.00	0.00
SO4-2	0.00	0.00	0.00	0.01	0.03	-	0.00	0.00	0.00	0.03
Total Flow kmol/sec	0.08	0.08	0.08	1.23	1.23	0.07	0.07	0.07	0.07	1.16
Total Flow kg/sec	1.39	1.39	1.39	62.15	62.15	1.25	1.25	1.25	1.25	60.90
Total Flow cum/sec	2.73	2.46	0.00	0.05	9.43	8.47	7.47	0.00	0.00	0.04
Temperature K	430.00	390.00	343.00	472.00	441.75	441.00	390.00	313.00	313.00	441.00
Pressure bar	1.00	1.00	1.00	1.00	0.30	0.30	0.30	0.30	0.30	0.30
Vapor Frac	1.00	1.00	-	-	0.06	1.00	1.00	-	-	-
Liquid Frac	0.00	0.00	1.00	1.00	0.94	-	0.00	1.00	1.00	1.00

Table 34: Mass Balance for Case 1

	436	437	438	439	440	441	442	443	444	445
To	HX-126	FL-113	PP-104	HX-127	FL-114	HX-128	MX-105	FL-115	CO-104	MX-105
From	VL-106	HX-126	FL-113	PP-104	HX-127	FL-114	FL-114	HX-128	FL-115	FL-115
	MIXED	LIQUID	LIQUID	LIQUID	MIXED	VAPOR	LIQUID	MIXED	VAPOR	LIQUID
Substream: MIXED										
Mole Flow kmol/sec										
H2O	0.32	0.25	0.41	0.41	1.21	0.93	0.28	0.92	0.92	0.01
H2SO4	0.16	0.09	0.65	0.65	1.39	0.12	1.28	0.12	0.10	0.03
H2	-	-	-	-	-	-	-	-	-	-
O2	-	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO3	0.00	0.00	0.00	0.00	0.03	0.03	0.00	0.02	0.02	0.00
OH-	0.00	0.00	0.00	0.00	0.00	-	0.00	0.00	-	0.00
HSO3-	0.00	0.00	0.00	0.00	0.00	-	0.00	0.00	-	0.00
HSO4-	0.34	0.41	0.81	0.81	0.05	-	0.05	0.00	-	0.00
H3O+	0.34	0.41	0.82	0.82	0.05	-	0.05	0.00	-	0.00
SO3-2	0.00	0.00	0.00	0.00	0.00	-	0.00	0.00	-	0.00
SO4-2	0.00	0.00	0.00	0.00	0.00	-	0.00	0.00	-	0.00
Mass Flow kg/sec										
H2O	5.75	4.44	7.44	7.44	21.87	16.81	5.07	16.64	16.53	0.11
H2SO4	15.62	8.65	64.11	64.11	136.73	11.46	125.28	12.14	9.59	2.55
H2	-	-	-	-	-	-	-	-	-	-
O2	-	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO2	0.00	0.00	0.08	0.08	0.08	0.08	0.00	0.08	0.08	0.00
SO3	0.00	0.00	0.00	0.00	2.33	2.30	0.03	1.66	1.66	0.00
OH-	0.00	0.00	0.00	0.00	0.00	-	0.00	0.00	-	0.00
HSO3-	0.00	0.00	0.00	0.00	0.00	-	0.00	0.00	-	0.00
HSO4-	32.98	39.69	78.89	78.88	4.41	-	4.41	0.11	-	0.11
H3O+	6.49	7.88	15.55	15.55	0.86	-	0.86	0.02	-	0.02
SO3-2	0.00	0.00	0.00	0.00	0.00	-	0.00	0.00	-	0.00
SO4-2	0.06	0.25	0.23	0.23	0.00	-	0.00	0.00	-	0.00
Total Flow kmol/sec	1.16	1.16	2.70	2.70	2.73	1.08	1.65	1.07	1.04	0.03
Total Flow kg/sec	60.90	60.90	166.29	166.29	166.29	30.64	135.65	30.64	27.86	2.79
Total Flow cum/sec	19.30	0.04	0.10	0.10	51.88	51.79	0.09	49.42	49.42	0.00
Temperature K	417.48	370.00	370.00	370.03	579.00	579.00	579.00	575.00	575.00	575.00
Pressure bar	0.10	0.10	0.10	1.00	1.00	1.00	1.00	1.00	1.00	1.00
Vapor Frac	0.05	-	-	-	0.40	1.00	-	0.97	1.00	-
Liquid Frac	0.95	1.00	1.00	1.00	0.60	-	1.00	0.03	-	1.00

Table 35: Mass Balance for Case 1

	446	447	448	FEED-H2O
To	HX-129	HX-130	PP-103	MX-104
From	MX-105	HX-129	FL-107	
	MIXED	LIQUID	LIQUID	LIQUID
Substream: MIXED				
Mole Flow kmol/sec				
H2O	0.29	0.27	0.00	0.96
H2SO4	1.30	1.28	0.00	0.00
H2	-	-	-	-
O2	-	-	0.00	-
SO2	0.00	0.00	0.00	-
SO3	0.00	0.00	0.00	0.00
OH-	0.00	0.00	0.00	0.00
HSO3-	0.00	0.00	0.00	-
HSO4-	0.05	0.07	0.00	0.00
H3O+	0.05	0.07	0.00	0.00
SO3-2	0.00	0.00	0.00	-
SO4-2	0.00	0.00	0.00	0.00
Mass Flow kg/sec				
H2O	5.18	4.82	0.00	17.38
H2SO4	127.83	125.90	0.00	0.00
H2	-	-	-	-
O2	-	-	0.00	-
SO2	0.00	0.00	0.00	-
SO3	0.03	0.01	0.00	0.00
OH-	0.00	0.00	0.00	0.00
HSO3-	0.00	0.00	0.00	-
HSO4-	4.52	6.44	0.00	0.01
H3O+	0.89	1.26	0.00	0.00
SO3-2	0.00	0.00	0.00	-
SO4-2	0.00	0.00	0.00	0.00
Total Flow kmol/sec	1.68	1.68	0.00	0.97
Total Flow kg/sec	138.44	138.44	0.00	17.39
Total Flow cum/sec	0.09	0.09	0.00	0.02
Temperature K	578.92	550.00	343.00	373.15
Pressure bar	1.00	1.00	1.00	21.00
Vapor Frac	0.00	-	-	-
Liquid Frac	1.00	1.00	1.00	1.00

Mass Balance: Case 2

Table 36: Mass Balance for Case 2

Stream No	101	102	103	104	105	106	107	108	109	110	111	112
Temperature K	439	502.5	503.4	500	600	775	775	823.1	1093.2	1143.2	850	850
Pressure bar	1	15	40	40	40	40	40	40	40	40	40	40
Vapor Frac	0.066	0	0	0	0	1	1	1	1	1	1	1
Mole Flow kmol/sec	1.688	1.688	1.688	1.688	1.688	2.119	2.119	2.377	2.986	3.359	3.153	3.153
Mass Flow kg/sec	138.491	138.491	138.491	138.491	138.491	138.491	138.491	138.491	138.491	138.491	138.491	138.491
Volume Flow cum/sec	4.163	0.098	0.099	0.098	0.109	2.924	2.924	3.752	6.711	7.94	5.422	5.422
Mass Flow kg/sec												
SO3	0	0	0	0	0	34.507	34.507	55.186	103.947	48.466	32.009	32.009
SO2	0	0	0	0	0	0	0	0	0	45.509	45.509	45.509
O2	0	0	0	0	0	0	0	0	0	11.365	11.365	11.365
H2SO4	132.407	132.407	132.407	132.407	132.407	90.136	90.136	64.803	5.071	3.364	23.524	23.524
H2O	6.084	6.084	6.084	6.084	6.084	13.848	13.848	18.501	29.473	29.787	26.084	26.084
H2	0	0	0	0	0	0	0	0	0	0	0	0
Mole Flow kmol/sec												
SO3	0	0	0	0	0	0.431	0.431	0.689	1.298	0.605	0.4	0.4
SO2	0	0	0	0	0	0	0	0	0	0.71	0.71	0.71
O2	0	0	0	0	0	0	0	0	0	0.355	0.355	0.355
H2SO4	1.35	1.35	1.35	1.35	1.35	0.919	0.919	0.661	0.052	0.034	0.24	0.24
H2O	0.338	0.338	0.338	0.338	0.338	0.769	0.769	1.027	1.636	1.653	1.448	1.448
H2	0	0	0	0	0	0	0	0	0	0	0	0

Table 37: Mass Balance for Case 2

Stream No	113	201	202	203	204	205	206	207	208	209	210	211	212	213	214	215
	HX-104	HX-104	HX-105	HX-106	HX-106	FL-101	FL-101	FL-101	CO-101	CO-101	HX-107	HX-108	MX-101	MX-101	HX-109	FL-102
	VL-101	CO-104	HX-104	HX-105	PP-103	HX-106	HX-136	HX-134	FL-101	FL-104	CO-101	HX-107	HX-108	FL-108	MX-101	HX-109
	VAPOR	VAPOR	MIXED	MIXED	LIQUID	MIXED	MIXED	MIXED	VAPOR	VAPOR	VAPOR	MIXED	MIXED	VAPOR	MIXED	MIXED
Substream: MIXED																
Temperature K	783.01	752.74	613.15	573.15	343.09	393.15	393.00	393.00	393.15	560.00	823.12	600.00	500.00	373.00	477.11	313.15
Pressure bar	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00	21.00	21.00	21.00	21.00	21.00	21.00
Vapor Frac	1.00	1.00	0.88	0.74	-	0.29	0.28	1.00	1.00	1.00	1.00	0.99	0.97	1.00	0.97	0.16
Liquid Frac	-	-	0.12	0.26	1.00	0.71	0.72	0.00	-	-	-	0.01	0.03	-	0.03	0.84
Mole Flow kmol/sec																
H2O	1.65	1.12	2.24	2.06	0.09	1.46	0.14	0.00	0.15	1.63	1.78	1.78	1.77	0.04	1.81	1.74
H2SO4	0.03	0.12	0.69	0.69	0.00	0.03	0.00	0.00	0.00	0.02	0.02	0.01	0.00	0.00	0.00	0.00
H2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O2	0.36	0.00	0.36	0.36	0.00	0.36	0.00	0.00	0.35	0.00	0.36	0.36	0.36	0.00	0.36	0.36
SO2	0.71	0.00	0.71	0.71	0.00	0.71	0.02	0.01	0.72	0.01	0.73	0.73	0.73	0.70	1.43	1.40
SO3	0.60	0.03	0.10	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00	0.00
OH-	-	-	0.00	0.00	0.00	0.00	0.00	0.00	-	-	-	0.00	0.00	-	0.00	0.00
HSO3-	-	-	0.00	0.00	0.00	0.00	0.00	0.00	-	-	-	0.00	0.00	-	0.00	0.03
HSO4-	-	-	0.00	0.09	0.01	0.75	0.00	0.00	-	-	-	0.00	0.02	-	0.02	0.00
H3O+	-	-	0.00	0.09	0.01	0.79	0.00	0.00	-	-	-	0.00	0.02	-	0.02	0.06
SO3-2	-	-	0.00	0.00	0.00	0.00	0.00	0.00	-	-	-	0.00	0.00	-	0.00	0.00
SO4-2	-	-	0.00	0.00	0.00	0.02	0.00	0.00	-	-	-	0.00	0.00	-	0.00	0.01
Mass Flow kg/sec																
H2O	29.78	20.19	40.38	37.19	1.65	26.31	2.60	0.00	2.70	29.45	32.14	32.08	31.83	0.77	32.60	31.29
H2SO4	3.34	11.71	67.27	67.82	0.00	2.72	0.00	0.00	0.00	1.64	1.64	1.37	0.09	0.00	0.04	0.00
H2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O2	11.36	0.00	11.36	11.36	0.00	11.36	0.00	0.00	11.36	0.00	11.36	11.36	11.36	0.07	11.43	11.43
SO2	45.49	0.08	45.56	45.56	0.03	45.60	1.00	0.35	46.17	0.78	46.95	46.95	46.95	44.55	91.50	89.67
SO3	48.43	2.02	7.83	0.53	0.00	0.00	0.00	0.00	0.00	0.05	0.05	0.02	0.00	-	0.00	0.00
OH-	-	-	0.00	0.00	0.00	0.00	0.00	0.00	-	-	-	0.00	0.00	-	0.00	0.00
HSO3-	-	-	0.00	0.00	0.00	0.00	0.00	0.00	-	-	-	0.00	0.00	-	0.00	2.31
HSO4-	-	-	0.00	8.31	0.91	72.48	0.00	0.00	-	-	-	0.30	1.59	-	1.63	0.23
H3O+	-	-	0.00	1.63	0.26	15.00	0.00	0.00	-	-	-	0.06	0.31	-	0.32	1.16
SO3-2	-	-	0.00	0.00	0.00	0.00	0.00	0.00	-	-	-	0.00	0.00	-	0.00	0.00
SO4-2	-	-	0.00	0.00	0.21	2.00	0.00	0.00	-	-	-	0.00	0.00	-	0.01	1.44
Total Flow kmol/sec	3.36	1.27	4.09	4.00	0.12	4.11	0.16	0.01	1.23	1.66	2.89	2.89	2.89	0.74	3.63	3.60
Total Flow kg/sec	138.40	34.00	172.40	172.40	3.06	175.47	3.60	0.36	60.22	31.92	92.14	92.14	92.14	45.39	137.53	137.53
Total Flow cum/sec	72.76	26.33	60.78	46.95	0.00	12.82	0.48	0.06	13.20	25.61	9.36	6.61	5.19	0.90	6.14	0.75

Table 38: Mass Balance for Case 2

Stream No	216	217	218	219	220	221	222	223	224	225	226	301	302	303	304	305
	HX-110	FL-103	DR-101		TK-101	TK-101	TK-101	HX-111	HX-112	FL-104	VL-105	EL-101	EL-101	EL-102	MX-102	MX-102
	FL-102	HX-110	FL-103	DR-101	DR-101	FL-103	FL-102	TK-101	FL-101	HX-112	FL-104	HX-111	MEM-101	EL-101	EL-102	MEM-101
	VAPOR	MIXED	VAPOR	VAPOR	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	MIXED	LIQUID	LIQUID	LIQUID	MIXED	VAPOR	LIQUID
Substream: MIXED																
Temperature K	313.00	250.00	250.00	250.00	250.00	250.00	313.00	308.60	393.15	560.00	560.00	373.15	373.15	373.15	373.15	373.15
Pressure bar	21.00	21.00	21.00	21.00	21.00	21.00	21.00	21.00	3.00	3.00	3.00	21.00	21.00	21.00	21.00	21.00
Vapor Frac	1.00	0.64	1.00	1.00	-	-	-	-	-	0.55	-	-	-	0.42	1.00	-
Liquid Frac	-	0.36	-	-	1.00	1.00	1.00	1.00	1.00	0.45	1.00	1.00	1.00	0.58	-	1.00
Mole Flow kmol/sec																
H2O	0.00	0.00	0.00	-	0.00	0.00	1.73	1.72	1.45	2.01	0.37	1.79	0.71	0.47	-	0.18
H2SO4	0.00	-	-	-	-	-	0.00	0.00	0.02	0.56	0.54	0.00	0.00	0.09	-	-
H2	-	-	-	-	-	-	-	-	-	-	-	-	0.00	0.71	0.71	-
O2	0.36	0.36	0.36	0.36	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00	-	-
SO2	0.22	0.22	0.02	-	0.02	0.21	1.18	1.39	0.01	0.01	0.00	1.42	-	0.72	-	-
SO3	0.00	-	-	-	-	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	-
OH-	-	0.00	-	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00
HSO3-	-	0.00	-	-	0.00	0.00	0.03	0.04	0.00	0.00	0.00	0.01	-	0.00	-	-
HSO4-	-	-	-	-	-	-	0.00	0.00	0.75	0.24	0.23	0.01	0.00	0.63	-	-
H3O+	-	0.00	-	-	0.00	0.00	0.06	0.07	0.79	0.24	0.23	0.03	0.00	0.65	-	0.00
SO3-2	-	0.00	-	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00	-	-
SO4-2	-	-	-	-	-	-	0.01	0.02	0.02	0.00	0.00	0.01	0.00	0.01	-	-
Mass Flow kg/sec																
H2O	0.05	0.02	0.00	-	0.00	0.02	31.24	31.01	26.10	36.19	6.72	32.19	12.79	8.42	-	3.20
H2SO4	0.00	-	-	-	-	-	0.00	0.00	2.34	54.86	53.07	0.00	0.00	8.49	-	-
H2	-	-	-	-	-	-	-	-	-	-	-	-	0.00	1.43	1.43	-
O2	11.37	11.37	11.36	11.36	-	0.01	0.05	0.07	0.00	0.00	0.00	0.07	-	0.07	-	-
SO2	14.25	14.21	1.00	-	1.00	13.21	75.41	89.20	0.78	0.78	0.00	90.97	-	46.01	-	-
SO3	0.00	-	-	-	-	-	0.00	0.00	0.00	0.05	0.00	0.00	0.00	0.00	-	-
OH-	-	0.00	-	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00
HSO3-	-	0.05	-	-	0.00	0.05	2.32	2.90	0.00	0.00	0.00	0.67	-	0.00	-	-
HSO4-	-	-	-	-	-	-	0.23	0.14	72.60	22.84	22.77	1.12	0.00	61.38	-	-
H3O+	-	0.01	-	-	0.00	0.01	1.16	1.31	15.12	4.48	4.46	0.60	0.00	12.35	-	0.00
SO3-2	-	0.00	-	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00	-	-
SO4-2	-	-	-	-	-	-	1.44	1.53	2.26	0.00	0.00	0.56	0.00	0.81	-	-
Total Flow kmol/sec	0.58	0.58	0.37	0.36	0.02	0.21	3.02	3.24	3.05	3.05	1.38	3.27	0.71	3.27	0.71	0.18
Total Flow kg/sec	25.67	25.67	12.36	11.36	1.00	13.31	111.85	126.17	119.20	119.20	87.03	126.17	12.79	138.96	1.43	3.20
Total Flow cum/sec	0.67	0.36	0.35	0.34	0.00	0.01	0.08	0.09	0.08	25.67	0.06	0.09	0.01	2.03	1.06	0.00

Table 39: Mass Balance for Case 2

Stream No	306	307	308	309	310	311	312	313	314	315	316	317	401	402	403	404
	HX-113	FL-105	HX-114	DR-102		MX-103	MX-103	HX-115	MX-104	MEM-101	VL-102	HX-116	FL-106	HX-117	FL-107	CO-102
	MX-102	HX-113	FL-105	HX-114	DR-102	DR-102	FL-105	MX-103	HX-115	MX-104	EL-102	VL-102	HX-116	FL-106	HX-117	FL-107
	MIXED	MIXED	VAPOR	MIXED	VAPOR	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	MIXED	MIXED	MIXED	VAPOR	MIXED	VAPOR
Substream: MIXED																
Temperature K	352.95	348.15	348.15	313.15	313.15	313.15	348.15	345.49	373.15	373.15	373.15	348.81	365.00	365.00	343.00	343.00
Pressure bar	21.00	21.00	21.00	20.00	20.00	20.00	21.00	20.00	21.00	21.00	21.00	1.00	1.00	1.00	1.00	1.00
Vapor Frac	0.82	0.82	1.00	0.98	1.00	-	-	-	-	-	0.17	0.28	0.28	1.00	1.00	1.00
Liquid Frac	0.18	0.18	-	0.02	-	1.00	1.00	1.00	1.00	1.00	0.83	0.72	0.72	-	0.00	-
Mole Flow kmol/sec																
H2O	0.18	0.18	0.01	0.01	-	0.01	0.16	0.18	0.18	0.89	0.45	0.44	0.46	0.01	0.01	0.19
H2SO4	-	-	-	-	-	-	-	-	-	0.00	0.09	0.07	0.08	0.00	0.00	0.00
H2	0.71	0.71	0.71	0.71	0.71	-	0.00	0.00	0.00	0.00	-	-	-	-	-	-
O2	-	-	-	-	-	-	-	-	-	-	0.00	0.00	0.00	0.00	0.00	0.00
SO2	-	-	-	-	-	-	-	-	-	-	0.72	0.72	0.72	0.71	0.71	0.71
SO3	-	-	-	-	-	-	-	-	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-	0.00	0.00	-	0.00	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00	-
HSO3-	-	-	-	-	-	-	-	-	-	-	0.00	0.00	0.00	-	0.00	-
HSO4-	-	-	-	-	-	-	-	-	-	0.00	0.63	0.66	0.64	-	0.00	-
H3O+	0.00	0.00	-	0.00	-	0.00	0.00	0.00	0.00	0.00	0.66	0.67	0.65	-	0.00	-
SO3-2	-	-	-	-	-	-	-	-	-	-	0.00	0.00	0.00	-	0.00	-
SO4-2	-	-	-	-	-	-	-	-	-	0.00	0.02	0.01	0.01	-	0.00	-
Mass Flow kg/sec																
H2O	3.20	3.20	0.24	0.24	-	0.24	2.95	3.20	3.20	15.99	8.10	7.94	8.29	0.23	0.23	3.37
H2SO4	-	-	-	-	-	-	-	-	-	0.00	8.37	6.51	8.23	0.00	0.00	0.00
H2	1.43	1.43	1.43	1.43	1.43	-	0.00	0.00	0.00	0.00	-	-	-	-	-	-
O2	-	-	-	-	-	-	-	-	-	-	0.07	0.07	0.07	0.07	0.07	0.07
SO2	-	-	-	-	-	-	-	-	-	-	46.01	46.01	46.01	45.58	45.58	45.55
SO3	-	-	-	-	-	-	-	-	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-	0.00	0.00	-	0.00	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00	-
HSO3-	-	-	-	-	-	-	-	-	-	-	0.00	0.00	0.00	-	0.00	-
HSO4-	-	-	-	-	-	-	-	-	-	0.00	60.78	63.63	62.14	-	0.00	-
H3O+	0.00	0.00	-	0.00	-	0.00	0.00	0.00	0.00	0.00	12.64	12.80	12.43	-	0.00	-
SO3-2	-	-	-	-	-	-	-	-	-	-	0.00	0.00	0.00	-	0.00	-
SO4-2	-	-	-	-	-	-	-	-	-	0.00	1.85	0.85	0.64	-	0.00	-
Total Flow kmol/sec	0.89	0.89	0.72	0.72	0.71	0.01	0.16	0.18	0.18	0.89	2.56	2.56	2.56	0.73	0.73	0.90
Total Flow kg/sec	4.63	4.63	1.68	1.68	1.43	0.24	2.95	3.20	3.20	15.99	137.81	137.81	137.81	45.88	45.88	48.98
Total Flow cum/sec	1.03	1.01	1.01	0.94	0.94	0.00	0.00	0.00	0.00	0.02	0.62	20.67	21.94	21.88	20.53	25.41

Table 40: Mass Balance for Case 2

Stream No	405	406	407	408	409	410	411	412	413	414	415	416	417	418	419	420
	HX-118	FL-108	MX-106	PP-105	HX-135	HX-136	VL-103	FL-109	HX-119	FL-110	CO-103	HX-131	HX-132	HX-133	HX-134	VL-104
	CO-102	HX-118	FL-108	MX-106	PP-105	HX-135	FL-106	VL-103	FL-109	HX-119	FL-110	CO-103	HX-131	HX-132	HX-133	FL-109
	VAPOR	MIXED	LIQUID	MIXED	MIXED	MIXED	LIQUID	MIXED	VAPOR	MIXED	VAPOR	VAPOR	VAPOR	VAPOR	VAPOR	LIQUID
Substream: MIXED																
Temperature K	716.76	373.00	373.00	320.26	376.72	350.00	365.00	364.49	325.00	313.00	313.00	752.97	685.00	645.00	600.00	325.00
Pressure bar	21.00	21.00	21.00	0.30	0.30	0.30	1.00	0.30	0.30	0.30	0.30	3.00	3.00	3.00	3.00	0.30
Vapor Frac	1.00	0.82	-	0.15	0.15	0.10	-	0.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	-
Liquid Frac	-	0.18	1.00	0.85	0.85	0.90	1.00	1.00	-	0.00	-	-	-	-	-	1.00
Mole Flow kmol/sec																
H2O	0.19	0.19	0.14	0.14	0.14	0.14	0.45	0.45	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.41
H2SO4	0.00	0.00	0.00	0.00	0.00	0.00	0.08	0.08	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.05
H2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO2	0.71	0.71	0.02	0.02	0.02	0.02	0.01	0.01	0.00	0.00	0.00	0.01	0.01	0.01	0.01	0.00
SO3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00	-	-	-	-	-	0.00
HSO3-	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00	-	-	-	-	-	0.00
HSO4-	-	0.00	0.00	0.00	0.00	0.00	0.64	0.64	-	0.00	-	-	-	-	-	0.67
H3O+	-	0.00	0.00	0.00	0.00	0.00	0.65	0.65	-	0.00	-	-	-	-	-	0.69
SO3-2	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00	-	-	-	-	-	0.00
SO4-2	-	0.00	0.00	0.00	0.00	0.00	0.01	0.01	-	0.00	-	-	-	-	-	0.01
Mass Flow kg/sec																
H2O	3.37	3.35	2.58	2.59	2.59	2.59	8.06	8.05	0.00	0.00	0.00	0.00	0.00	0.00	0.00	7.38
H2SO4	0.00	0.00	0.00	0.00	0.00	0.00	8.23	8.18	0.00	0.00	0.00	0.00	0.00	0.00	0.00	4.83
H2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O2	0.07	0.07	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO2	45.55	45.52	0.97	0.99	0.99	0.99	0.43	0.43	0.15	0.15	0.15	0.35	0.35	0.35	0.35	0.28
SO3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00	-	-	-	-	-	0.00
HSO3-	-	0.03	0.03	0.01	0.01	0.02	0.00	0.00	-	0.00	-	-	-	-	-	0.00
HSO4-	-	0.00	0.00	0.00	0.00	0.00	62.14	62.20	-	0.00	-	-	-	-	-	65.18
H3O+	-	0.01	0.01	0.00	0.00	0.00	12.43	12.44	-	0.00	-	-	-	-	-	13.15
SO3-2	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00	-	-	-	-	-	0.00
SO4-2	-	0.00	0.00	0.00	0.00	0.00	0.64	0.63	-	0.00	-	-	-	-	-	0.96
Total Flow kmol/sec	0.90	0.90	0.16	0.16	0.16	0.16	1.84	1.84	0.00	0.00	0.00	0.01	0.01	0.01	0.01	1.84
Total Flow kg/sec	48.98	48.98	3.60	3.60	3.60	3.60	91.93	91.93	0.15	0.15	0.15	0.36	0.36	0.36	0.36	91.78
Total Flow cum/sec	2.53	0.91	0.00	2.09	0.25	0.15	0.06	0.57	0.21	0.20	0.20	0.12	0.11	0.10	0.09	0.05

Table 41: Mass Balance for Case 2

Stream No	421	422	423	424	425	426	427	428	429	430	431	432	433	434	435	436
	HX-120	FL-113	FL-111	HX-121	HX-122	HX-123	FL-107	VL-106	FL-112	HX-124	HX-125	FL-110	MX-106	VL-107	HX-126	FL-113
	VL-104	HX-120	VL-105	FL-111	HX-121	HX-122	HX-123	FL-111	VL-106	FL-112	HX-124	HX-125	FL-110	FL-112	VL-107	HX-126
	MIXED	MIXED	MIXED	VAPOR	MIXED	MIXED	LIQUID	LIQUID	MIXED	MISSING	MISSING	MISSING	LIQUID	LIQUID	MIXED	LIQUID
Substream: MIXED																
Temperature K	324.65	370.00	523.09	550.00	430.00	390.00	343.00	550.00	516.33				313.00	471.00	470.63	370.00
Pressure bar	0.10	0.10	1.00	1.00	1.00	1.00	1.00	1.00	0.30	0.30	0.30	0.30	0.30	0.30	0.10	0.10
Vapor Frac	0.00	0.00	0.05	1.00	0.86	0.71	-	-	0.06				-	-	0.00	-
Liquid Frac	1.00	1.00	0.95	-	0.14	0.29	1.00	1.00	0.94				1.00	1.00	1.00	1.00
Mole Flow kmol/sec																
H2O	0.41	0.45	0.38	0.28	0.27	0.27	0.27	0.23	0.24	-	-	-	0.00	0.19	0.19	0.14
H2SO4	0.05	0.09	0.55	0.01	0.00	0.00	0.00	0.66	0.68	-	-	-	0.00	0.62	0.62	0.57
H2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	-	-	0.00	0.00	0.00	0.00
SO2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	-	-	0.00	0.00	0.00	0.00
SO3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	-	-	0.00	0.00	0.00	0.00
OH-	0.00	0.00	0.00	-	0.00	0.00	0.00	0.00	0.00	-	-	-	0.00	0.00	0.00	0.00
HSO3-	0.00	0.00	0.00	-	0.00	0.00	0.00	0.00	0.00	-	-	-	0.00	0.00	0.00	0.00
HSO4-	0.67	0.64	0.23	-	0.01	0.01	0.01	0.10	0.08	-	-	-	0.00	0.14	0.14	0.19
H3O+	0.69	0.65	0.23	-	0.01	0.01	0.01	0.10	0.08	-	-	-	0.00	0.14	0.14	0.19
SO3-2	0.00	0.00	0.00	-	0.00	0.00	0.00	0.00	0.00	-	-	-	0.00	0.00	0.00	0.00
SO4-2	0.01	0.01	0.00	-	0.00	0.00	0.00	0.00	0.00	-	-	-	0.00	0.00	0.00	0.00
Mass Flow kg/sec																
H2O	7.37	8.18	6.85	5.05	4.83	4.81	4.81	4.09	4.40	-	-	-	0.00	3.41	3.41	2.46
H2SO4	4.81	8.80	53.77	1.05	0.08	0.00	0.00	64.98	66.62	-	-	-	0.00	61.26	61.29	56.11
H2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
O2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	-	-	0.00	0.00	0.00	0.00
SO2	0.28	0.28	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	-	-	0.00	0.00	0.00	0.00
SO3	0.00	0.00	0.00	0.07	0.00	0.00	0.00	0.00	0.02	-	-	-	0.00	0.00	0.00	0.00
OH-	0.00	0.00	0.00	-	0.00	0.00	0.00	0.00	0.00	-	-	-	0.00	0.00	0.00	0.00
HSO3-	0.00	0.00	0.00	-	0.00	0.00	0.00	0.00	0.00	-	-	-	0.00	0.00	0.00	0.00
HSO4-	65.22	61.65	22.08	-	1.04	1.05	1.04	9.86	8.22	-	-	-	0.00	13.55	13.52	18.63
H3O+	13.16	12.30	4.33	-	0.21	0.23	0.24	1.93	1.61	-	-	-	0.00	2.66	2.65	3.66
SO3-2	0.00	0.00	0.00	-	0.00	0.00	0.00	0.00	0.00	-	-	-	0.00	0.00	0.00	0.00
SO4-2	0.94	0.56	0.00	-	0.01	0.07	0.08	0.00	0.00	-	-	-	0.00	0.00	0.00	0.01
Total Flow kmol/sec	1.84	1.84	1.38	0.29	0.29	0.29	0.29	1.09	1.09	-	-	-	0.00	1.09	1.09	1.09
Total Flow kg/sec	91.78	91.78	87.03	6.17	6.17	6.17	6.17	80.87	80.87	-	-	-	0.00	80.87	80.87	80.87
Total Flow cum/sec	0.86	1.60	3.27	13.29	8.86	6.59	0.01	0.05	9.90	-	-	-	0.00	0.05	0.37	0.05

Table 42: Mass Balance for Case 2

Stream No	437	438	439	440	441	442	443	444	445	446	447	448	FEED-H2O
	PP-104	HX-127	FL-114	HX-128	FL-115	CO-104	MX-105	MX-105	HX-129	HX-130	PP-103	CO-103	MX-104
	FL-113	PP-104	HX-127	FL-114	HX-128	FL-115	FL-114	FL-115	MX-105	HX-129	FL-107	FL-113	
	LIQUID	LIQUID	MIXED	VAPOR	MIXED	VAPOR	LIQUID	LIQUID	MIXED	LIQUID	LIQUID	VAPOR	LIQUID
Substream: MIXED													
Temperature K	370.00	370.03	579.00	579.00	575.00	575.00	579.00	575.00	578.90	550.00	343.00	370.00	373.15
Pressure bar	0.10	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	0.10	21.00
Vapor Frac	-	-	0.45	1.00	0.97	1.00	-	-	0.00	-	-	1.00	-
Liquid Frac	1.00	1.00	0.55	-	0.03	-	1.00	1.00	1.00	1.00	1.00	-	1.00
Mole Flow kmol/sec													
H2O	0.47	0.47	1.42	1.14	1.13	1.12	0.28	0.01	0.29	0.27	0.09	0.00	0.71
H2SO4	0.54	0.54	1.41	0.14	0.15	0.12	1.27	0.03	1.30	1.28	0.00	0.00	0.00
H2	-	-	-	-	-	-	-	-	-	-	-	-	-
O2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-
SO2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-
SO3	0.00	0.00	0.04	0.04	0.03	0.03	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-	0.00	0.00	0.00	-	0.00	-	0.00	0.00	0.00	0.00	0.00	-	0.00
HSO3-	0.00	0.00	0.00	-	0.00	-	0.00	0.00	0.00	0.00	0.00	-	-
HSO4-	0.95	0.95	0.05	-	0.00	-	0.05	0.00	0.05	0.07	0.01	-	0.00
H3O+	0.96	0.96	0.05	-	0.00	-	0.05	0.00	0.05	0.07	0.01	-	0.00
SO3-2	0.00	0.00	0.00	-	0.00	-	0.00	0.00	0.00	0.00	0.00	-	-
SO4-2	0.00	0.00	0.00	-	0.00	-	0.00	0.00	0.00	0.00	0.00	-	0.00
Mass Flow kg/sec													
H2O	8.54	8.54	25.57	20.53	20.33	20.19	5.05	0.13	5.18	4.82	1.65	0.00	12.79
H2SO4	53.24	53.24	138.70	13.99	14.82	11.71	124.71	3.11	127.82	125.90	0.00	0.00	0.00
H2	-	-	-	-	-	-	-	-	-	-	-	-	-
O2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-
SO2	0.08	0.08	0.08	0.08	0.08	0.08	0.00	0.00	0.00	0.00	0.03	0.20	-
SO3	0.00	0.00	2.84	2.81	2.02	2.02	0.03	0.00	0.03	0.01	0.00	0.00	0.00
OH-	0.00	0.00	0.00	-	0.00	-	0.00	0.00	0.00	0.00	0.00	-	0.00
HSO3-	0.00	0.00	0.00	-	0.00	-	0.00	0.00	0.00	0.00	0.00	-	-
HSO4-	92.10	92.09	4.39	-	0.13	-	4.39	0.13	4.53	6.44	0.91	-	0.00
H3O+	18.17	18.17	0.86	-	0.03	-	0.86	0.03	0.89	1.26	0.26	-	0.00
SO3-2	0.00	0.00	0.00	-	0.00	-	0.00	0.00	0.00	0.00	0.00	-	-
SO4-2	0.32	0.32	0.00	-	0.00	-	0.00	0.00	0.00	0.00	0.21	-	0.00
Total Flow kmol/sec	2.93	2.93	2.96	1.32	1.31	1.27	1.64	0.04	1.68	1.68	0.12	0.00	0.71
Total Flow kg/sec	172.44	172.44	172.44	37.41	37.41	34.00	135.04	3.40	138.44	138.44	3.06	0.21	12.79
Total Flow cum/sec	0.10	0.10	63.33	63.24	60.35	60.35	0.09	0.00	0.09	0.09	0.00	1.04	0.01

Mass Balance: Case 3

Table 43: Mass Balance for Case 3

Stream No	101	102	103	104	105	106	107	108	109	110	111	112
Temperature K	439.00	530.10	532.30	579.00	610.00	823.00	823.00	823.10	1,028.20	1,143.20	911.70	911.70
Pressure bar	1.00	40.00	90.00	90.00	90.00	90.00	90.00	90.00	90.00	90.00	90.00	90.00
Vapor Frac	0.07	-	-	-	-	1.00	1.00	1.00	1.00	1.00	1.00	1.00
Mole Flow kmol/sec	1.69	1.69	1.69	1.69	1.69	2.20	2.20	2.21	2.86	3.26	3.07	3.07
Mass Flow kg/sec	138.49	138.49	138.49	138.49	138.49	138.49	138.49	138.49	138.49	138.49	138.49	138.49
Volume Flow cum/sec	4.41	0.10	0.10	0.11	0.11	1.68	1.68	1.68	2.71	3.40	2.58	2.58
Mass Flow kg/sec												
SO3	-	-	-	-	-	41.38	41.38	41.43	93.61	55.67	40.33	40.33
SO2	-	-	-	-	-	-	-	-	-	37.31	37.31	37.31
O2	-	-	-	-	-	-	-	-	-	9.32	9.32	9.32
H2SO4	132.41	132.41	132.41	132.41	132.41	81.71	81.71	81.65	17.74	7.09	25.88	25.88
H2O	6.08	6.08	6.08	6.08	6.08	15.39	15.39	15.40	27.14	29.10	25.65	25.65
H2	-	-	-	-	-	-	-	-	-	-	-	-
Mole Flow kmol/sec												
SO3	-	-	-	-	-	0.52	0.52	0.52	1.17	0.70	0.50	0.50
SO2	-	-	-	-	-	-	-	-	-	0.58	0.58	0.58
O2	-	-	-	-	-	-	-	-	-	0.29	0.29	0.29
H2SO4	1.35	1.35	1.35	1.35	1.35	0.83	0.83	0.83	0.18	0.07	0.26	0.26
H2O	0.34	0.34	0.34	0.34	0.34	0.85	0.85	0.86	1.51	1.62	1.42	1.42
H2	-	-	-	-	-	-	-	-	-	-	-	-

Table 44: Mass Balance for Case 3

Stream No	113	201	202	203	204	205	206	207	208	209
	HX-104	HX-104	HX-105	HX-106	HX-106	FL-101	FL-101	FL-101	CO-101	CO-101
	VL-101	CO-104	HX-104	HX-105	PP-103	HX-106	HX-136	HX-134	FL-101	FL-104
	VAPOR	VAPOR	MIXED	MIXED	LIQUID	MIXED	MIXED	MIXED	VAPOR	VAPOR
Substream: MIXED										
Temperature K	811.92	752.75	613.15	573.15	343.07	393.15	393.00	393.00	393.15	560.00
Pressure bar	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00
Vapor Frac	1.00	1.00	0.82	0.68	-	0.23	0.28	1.00	1.00	1.00
Liquid Frac	-	-	0.18	0.32	1.00	0.77	0.72	0.00	-	-
Mole Flow kmol/sec										
H2O	1.66	1.17	2.15	1.96	0.15	1.33	0.15	0.00	0.09	1.57
H2SO4	0.03	0.12	0.83	0.80	0.00	0.05	0.00	0.00	0.00	0.02
H2	-	-	-	-	-	-	-	-	-	-
O2	0.29	0.00	0.29	0.29	0.00	0.29	0.00	0.00	0.29	0.00
SO2	0.58	0.00	0.58	0.58	0.00	0.58	0.02	0.00	0.59	0.01
SO3	0.74	0.03	0.08	0.01	0.00	0.00	0.00	0.00	0.00	0.00
OH-	-	-	0.00	0.00	0.00	0.00	0.00	0.00	-	-
HSO3-	-	-	0.00	0.00	0.00	0.00	0.00	0.00	-	-
HSO4-	-	-	0.00	0.11	0.01	0.87	0.00	0.00	-	-
H3O+	-	-	0.00	0.11	0.02	0.90	0.00	0.00	-	-
SO3-2	-	-	0.00	0.00	0.00	0.00	0.00	0.00	-	-
SO4-2	-	-	0.00	0.00	0.00	0.02	0.00	0.00	-	-
Mass Flow kg/sec										
H2O	29.91	21.05	38.65	35.27	2.70	23.90	2.65	0.00	1.56	28.34
H2SO4	2.62	12.21	81.86	78.69	0.00	4.67	0.00	0.00	0.00	1.58
H2	-	-	-	-	-	-	-	-	-	-
O2	9.31	0.00	9.31	9.31	0.00	9.31	0.00	0.00	9.31	0.00
SO2	37.29	0.08	37.36	37.36	0.05	37.41	1.02	0.29	37.86	0.86
SO3	59.27	2.11	6.66	0.44	0.00	0.00	0.00	0.00	0.00	0.05
OH-	-	-	0.00	0.00	0.00	0.00	0.00	0.00	-	-
HSO3-	-	-	0.00	0.00	0.00	0.00	0.00	0.00	-	-
HSO4-	-	-	0.00	10.68	1.12	84.11	0.00	0.00	-	-
H3O+	-	-	0.00	2.09	0.30	17.14	0.00	0.00	-	-
SO3-2	-	-	0.00	0.00	0.00	0.00	0.00	0.00	-	-
SO4-2	-	-	0.00	0.00	0.20	1.66	0.00	0.00	-	-
Total Flow kmol/sec	3.30	1.32	3.94	3.86	0.18	4.03	0.16	0.00	0.97	1.60
Total Flow kg/sec	138.40	35.44	173.84	173.84	4.36	178.21	3.67	0.30	48.73	30.83
Total Flow cum/sec	74.19	27.44	54.30	41.22	0.00	10.16	0.49	0.05	10.44	24.67

Table 45: Mass Balance for Case 3

Stream No	210	211	212	213	214	215	216	217	218	219
	HX-107	HX-108	MX-101	MX-101	HX-109	FL-102	HX-110	FL-103	DR-101	
	CO-101	HX-107	HX-108	FL-108	MX-101	HX-109	FL-102	HX-110	FL-103	DR-101
	VAPOR	MIXED	MIXED	VAPOR	MIXED	MIXED	VAPOR	MIXED	VAPOR	VAPOR
Substream: MIXED										
Temperature K	836.41	600.00	500.00	373.00	479.30	313.15	313.00	250.00	250.00	250.00
Pressure bar	21.00	21.00	21.00	21.00	21.00	21.00	21.00	21.00	21.00	21.00
Vapor Frac	1.00	0.99	0.96	1.00	0.96	0.16	1.00	0.62	1.00	1.00
Liquid Frac	-	0.01	0.04	-	0.04	0.84	-	0.38	-	-
Mole Flow kmol/sec										
H2O	1.66	1.66	1.64	0.03	1.68	1.62	0.00	0.00	0.00	-
H2SO4	0.02	0.01	0.00	0.00	0.00	0.00	0.00	-	-	-
H2	-	-	-	-	-	-	-	-	-	-
O2	0.29	0.29	0.29	0.00	0.29	0.29	0.29	0.29	0.29	0.29
SO2	0.60	0.60	0.60	0.57	1.17	1.15	0.20	0.20	0.01	-
SO3	0.00	0.00	0.00	-	0.00	0.00	0.00	-	-	-
OH-	-	0.00	0.00	-	0.00	0.00	-	0.00	-	-
HSO3-	-	0.00	0.00	-	0.00	0.02	-	0.00	-	-
HSO4-	-	0.00	0.02	-	0.02	0.00	-	-	-	-
H3O+	-	0.00	0.02	-	0.02	0.05	-	0.00	-	-
SO3-2	-	0.00	0.00	-	0.00	0.00	-	0.00	-	-
SO4-2	-	0.00	0.00	-	0.00	0.01	-	-	-	-
Mass Flow kg/sec										
H2O	29.90	29.83	29.60	0.63	30.22	29.12	0.04	0.02	0.00	-
H2SO4	1.58	1.28	0.08	0.00	0.04	0.00	0.00	-	-	-
H2	-	-	-	-	-	-	-	-	-	-
O2	9.31	9.31	9.31	0.06	9.37	9.37	9.32	9.32	9.31	9.31
SO2	38.72	38.72	38.72	36.28	75.00	73.50	12.54	12.51	0.82	-
SO3	0.05	0.02	0.00	-	0.00	0.00	0.00	-	-	-
OH-	-	0.00	0.00	-	0.00	0.00	-	0.00	-	-
HSO3-	-	0.00	0.00	-	0.00	1.89	-	0.04	-	-
HSO4-	-	0.34	1.54	-	1.57	0.28	-	-	-	-
H3O+	-	0.07	0.30	-	0.31	1.03	-	0.01	-	-
SO3-2	-	0.00	0.00	-	0.00	0.00	-	0.00	-	-
SO4-2	-	0.00	0.00	-	0.01	1.33	-	-	-	-
Total Flow kmol/sec	2.57	2.57	2.57	0.60	3.17	3.15	0.49	0.49	0.30	0.29
Total Flow kg/sec	79.56	79.56	79.56	36.96	116.52	116.52	21.91	21.91	10.14	9.31
Total Flow cum/sec	8.46	5.87	4.59	0.74	5.37	0.63	0.56	0.30	0.29	0.28

Table 46: Mass Balance for Case 3

Stream No	220	221	222	223	224	225	226	301	302	303
	TK-101	TK-101	TK-101	HX-111	HX-112	FL-104	VL-105	EL-101	EL-101	EL-102
	DR-101	FL-103	FL-102	TK-101	FL-101	HX-112	FL-104	HX-111	MEM-101	EL-101
	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID	MIXED	LIQUID	LIQUID	LIQUID	MIXED
Substream: MIXED										
Temperature K	250.00	250.00	313.00	308.48	393.15	560.00	560.00	373.15	373.15	373.15
Pressure bar	21.00	21.00	21.00	21.00	3.00	3.00	3.00	21.00	21.00	21.00
Vapor Frac	-	-	-	-	-	0.50	-	-	-	0.39
Liquid Frac	1.00	1.00	1.00	1.00	1.00	0.50	1.00	1.00	1.00	0.61
Mole Flow kmol/sec										
H2O	0.00	0.00	1.61	1.60	1.38	2.01	0.44	1.66	0.58	0.54
H2SO4	-	-	0.00	0.00	0.04	0.65	0.64	0.00	0.00	0.04
H2	-	-	-	-	-	-	-	-	0.00	0.58
O2	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00
SO2	0.01	0.18	0.95	1.14	0.01	0.01	0.00	1.16	-	0.59
SO3	-	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HSO3-	0.00	0.00	0.02	0.03	0.00	0.00	0.00	0.01	-	0.00
HSO4-	-	-	0.00	0.00	0.87	0.28	0.28	0.01	0.00	0.55
H3O+	0.00	0.00	0.05	0.06	0.91	0.28	0.28	0.03	0.00	0.57
SO3-2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00
SO4-2	-	-	0.01	0.01	0.02	0.00	0.00	0.00	0.00	0.01
Mass Flow kg/sec										
H2O	0.00	0.02	29.08	28.87	24.82	36.26	7.89	29.88	10.45	9.73
H2SO4	-	-	0.00	0.00	3.97	64.18	62.30	0.00	0.00	4.05
H2	-	-	-	-	-	-	-	-	0.00	1.17
O2	-	0.01	0.04	0.06	0.00	0.00	0.00	0.06	-	0.06
SO2	0.82	11.69	60.95	73.08	0.86	0.86	0.00	74.56	-	37.72
SO3	-	-	0.00	0.00	0.00	0.05	0.00	0.00	0.00	0.00
OH-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HSO3-	0.00	0.04	1.90	2.42	0.00	0.00	0.00	0.55	-	0.00
HSO4-	-	-	0.28	0.17	84.53	26.83	26.70	1.15	0.00	52.93
H3O+	0.00	0.01	1.03	1.17	17.33	5.26	5.23	0.54	0.00	10.84
SO3-2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00
SO4-2	-	-	1.33	1.44	1.94	0.00	0.00	0.47	0.00	1.17
Total Flow kmol/sec	0.01	0.18	2.66	2.85	3.23	3.23	1.62	2.88	0.58	2.88
Total Flow kg/sec	0.82	11.77	94.62	107.21	133.45	133.45	102.13	107.21	10.45	117.66
Total Flow cum/sec	0.00	0.01	0.07	0.08	0.09	24.74	0.07	0.08	0.01	1.66

Table 47: Mass Balance for Case 3

Stream No	304	305	306	307	308	309	310	311	312	313
	MX-102	MX-102	HX-113	FL-105	HX-114	DR-102		MX-103	MX-103	HX-115
	EL-102	MEM-101	MX-102	HX-113	FL-105	HX-114	DR-102	DR-102	FL-105	MX-103
	VAPOR	LIQUID	MIXED	MIXED	VAPOR	MIXED	VAPOR	LIQUID	LIQUID	LIQUID
Substream: MIXED										
Temperature K	373.15	373.15	350.11	348.15	348.15	313.15	313.15	313.15	348.15	342.12
Pressure bar	21.00	21.00	21.00	21.00	21.00	20.00	20.00	20.00	21.00	20.00
Vapor Frac	1.00	-	0.92	0.92	1.00	0.98	1.00	-	-	-
Liquid Frac	-	1.00	0.08	0.08	-	0.02	-	1.00	1.00	1.00
Mole Flow kmol/sec										
H2O	-	0.06	0.06	0.06	0.01	0.01	-	0.01	0.05	0.06
H2SO4	-	-	-	-	-	-	-	-	-	-
H2	0.58	-	0.58	0.58	0.58	0.58	0.58	-	0.00	0.00
O2	-	-	-	-	-	-	-	-	-	-
SO2	-	-	-	-	-	-	-	-	-	-
SO3	-	-	-	-	-	-	-	-	-	-
OH-	-	0.00	0.00	0.00	-	0.00	-	0.00	0.00	0.00
HSO3-	-	-	-	-	-	-	-	-	-	-
HSO4-	-	-	-	-	-	-	-	-	-	-
H3O+	-	0.00	0.00	0.00	-	0.00	-	0.00	0.00	0.00
SO3-2	-	-	-	-	-	-	-	-	-	-
SO4-2	-	-	-	-	-	-	-	-	-	-
Mass Flow kg/sec										
H2O	-	1.16	1.16	1.16	0.20	0.20	-	0.20	0.96	1.16
H2SO4	-	-	-	-	-	-	-	-	-	-
H2	1.17	-	1.17	1.17	1.17	1.17	1.17	-	0.00	0.00
O2	-	-	-	-	-	-	-	-	-	-
SO2	-	-	-	-	-	-	-	-	-	-
SO3	-	-	-	-	-	-	-	-	-	-
OH-	-	0.00	0.00	0.00	-	0.00	-	0.00	0.00	0.00
HSO3-	-	-	-	-	-	-	-	-	-	-
HSO4-	-	-	-	-	-	-	-	-	-	-
H3O+	-	0.00	0.00	0.00	-	0.00	-	0.00	0.00	0.00
SO3-2	-	-	-	-	-	-	-	-	-	-
SO4-2	-	-	-	-	-	-	-	-	-	-
Total Flow kmol/sec	0.58	0.06	0.65	0.65	0.59	0.59	0.58	0.01	0.05	0.06
Total Flow kg/sec	1.17	1.16	2.33	2.33	1.37	1.37	1.17	0.20	0.96	1.16
Total Flow cum/sec	0.87	0.00	0.83	0.83	0.83	0.77	0.77	0.00	0.00	0.00

Table 48: Mass Balance for Case 3

Stream No	314	315	316	317	401	402	403	404	405	406
	MX-104	MEM-101	VL-102	HX-116	FL-106	HX-117	FL-107	CO-102	HX-118	FL-108
	HX-115	MX-104	EL-102	VL-102	HX-116	FL-106	HX-117	FL-107	CO-102	HX-118
	LIQUID	LIQUID	MIXED	MIXED	MIXED	VAPOR	MIXED	VAPOR	VAPOR	MIXED
Substream: MIXED										
Temperature K	373.15	373.15	373.15	350.59	365.00	365.00	343.00	343.00	720.01	373.00
Pressure bar	21.00	21.00	21.00	1.00	1.00	1.00	1.00	1.00	21.00	21.00
Vapor Frac	-	-	0.16	0.26	0.26	1.00	1.00	1.00	1.00	0.79
Liquid Frac	1.00	1.00	0.84	0.74	0.74	-	0.00	-	-	0.21
Mole Flow kmol/sec										
H2O	0.06	0.64	0.52	0.53	0.54	0.02	0.02	0.18	0.18	0.18
H2SO4	-	0.00	0.04	0.03	0.04	0.00	0.00	0.00	0.00	0.00
H2	0.00	0.00	-	-	-	-	-	-	-	-
O2	-	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO2	-	-	0.59	0.59	0.59	0.58	0.58	0.58	0.58	0.58
SO3	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-	0.00	0.00	0.00	0.00	0.00	-	0.00	-	-	0.00
HSO3-	-	-	0.00	0.00	0.00	-	0.00	-	-	0.00
HSO4-	-	0.00	0.54	0.56	0.55	-	0.00	-	-	0.00
H3O+	0.00	0.00	0.59	0.58	0.57	-	0.00	-	-	0.00
SO3-2	-	-	0.00	0.00	0.00	-	0.00	-	-	0.00
SO4-2	-	0.00	0.02	0.01	0.01	-	0.00	-	-	0.00
Mass Flow kg/sec										
H2O	1.16	11.61	9.45	9.50	9.72	0.37	0.37	3.28	3.28	3.26
H2SO4	-	0.00	3.94	3.00	3.87	0.00	0.00	0.00	0.00	0.00
H2	0.00	0.00	-	-	-	-	-	-	-	-
O2	-	-	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06
SO2	-	-	37.71	37.71	37.71	37.34	37.34	37.29	37.29	37.27
SO3	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-	0.00	0.00	0.00	0.00	0.00	-	0.00	-	-	0.00
HSO3-	-	-	0.00	0.00	0.00	-	0.00	-	-	0.03
HSO4-	-	0.00	52.09	53.98	53.41	-	0.00	-	-	0.00
H3O+	0.00	0.00	11.13	11.08	10.85	-	0.00	-	-	0.01
SO3-2	-	-	0.00	0.00	0.00	-	0.00	-	-	0.00
SO4-2	-	0.00	2.21	1.27	0.98	-	0.00	-	-	0.00
Total Flow kmol/sec	0.06	0.64	2.30	2.30	2.30	0.61	0.61	0.77	0.77	0.77
Total Flow kg/sec	1.16	11.61	116.60	116.60	116.60	37.77	37.77	40.63	40.63	40.63
Total Flow cum/sec	0.00	0.01	0.52	17.19	18.28	18.23	17.10	21.62	2.16	0.74

Table 49: Mass Balance for Case 3

Stream No	407	408	409	410	411	412	413	414	415	416
	MX-106	PP-105	HX-135	HX-136	VL-103	FL-109	HX-119	FL-110	CO-103	HX-131
	FL-108	MX-106	PP-105	HX-135	FL-106	VL-103	FL-109	HX-119	FL-110	CO-103
	LIQUID	MIXED	MIXED	MIXED	LIQUID	MIXED	VAPOR	MIXED	VAPOR	VAPOR
Substream: MIXED										
Temperature K	373.00	320.26	376.72	350.00	365.00	364.41	325.00	313.00	313.00	754.09
Pressure bar	21.00	0.30	3.00	3.00	1.00	0.30	0.30	0.30	0.30	3.00
Vapor Frac	-	0.15	0.15	0.10	-	0.00	1.00	1.00	1.00	1.00
Liquid Frac	1.00	0.85	0.85	0.90	1.00	1.00	-	0.00	-	-
Mole Flow kmol/sec										
H2O	0.15	0.15	0.15	0.15	0.52	0.52	0.00	0.00	0.00	0.00
H2SO4	0.00	0.00	0.00	0.00	0.04	0.04	0.00	0.00	0.00	0.00
H2	-	-	-	-	-	-	-	-	-	-
O2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO2	0.02	0.02	0.02	0.02	0.01	0.01	0.00	0.00	0.00	0.00
SO3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00	-	-
HSO3-	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00	-	-
HSO4-	0.00	0.00	0.00	0.00	0.55	0.55	-	0.00	-	-
H3O+	0.00	0.00	0.00	0.00	0.57	0.57	-	0.00	-	-
SO3-2	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00	-	-
SO4-2	0.00	0.00	0.00	0.00	0.01	0.01	-	0.00	-	-
Mass Flow kg/sec										
H2O	2.64	2.65	2.65	2.64	9.35	9.34	0.00	0.00	0.00	0.00
H2SO4	0.00	0.00	0.00	0.00	3.87	3.84	0.00	0.00	0.00	0.00
H2	-	-	-	-	-	-	-	-	-	-
O2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO2	0.99	1.01	1.01	1.01	0.37	0.37	0.12	0.12	0.12	0.29
SO3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00	-	-
HSO3-	0.03	0.01	0.01	0.02	0.00	0.00	-	0.00	-	-
HSO4-	0.00	0.00	0.00	0.00	53.41	53.45	-	0.00	-	-
H3O+	0.01	0.00	0.00	0.00	10.85	10.86	-	0.00	-	-
SO3-2	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00	-	-
SO4-2	0.00	0.00	0.00	0.00	0.98	0.96	-	0.00	-	-
Total Flow kmol/sec	0.16	0.16	0.16	0.16	1.70	1.70	0.00	0.00	0.00	0.00
Total Flow kg/sec	3.67	3.67	3.67	3.67	78.83	78.83	0.12	0.12	0.12	0.30
Total Flow cum/sec	0.00	2.13	0.25	0.15	0.05	0.52	0.18	0.17	0.17	0.10

Table 50: Mass Balance for Case 3

Stream No	417	418	419	420	421	422	423	424	425	426
	HX-132	HX-133	HX-134	VL-104	HX-120	FL-113	FL-111	HX-121	HX-122	HX-123
	HX-131	HX-132	HX-133	FL-109	VL-104	HX-120	VL-105	FL-111	HX-121	HX-122
	VAPOR	VAPOR	VAPOR	LIQUID	MIXED	MIXED	MIXED	VAPOR	MIXED	MIXED
Substream: MIXED										
Temperature K	685.00	645.00	600.00	325.00	324.63	370.00	523.13	550.00	430.00	390.00
Pressure bar	3.00	3.00	3.00	0.30	0.10	0.10	1.00	1.00	1.00	1.00
Vapor Frac	1.00	1.00	1.00	-	0.00	0.00	0.05	1.00	0.86	0.71
Liquid Frac	-	-	-	1.00	1.00	1.00	0.95	-	0.14	0.29
Mole Flow kmol/sec										
H2O	0.00	0.00	0.00	0.49	0.49	0.52	0.45	0.33	0.31	0.31
H2SO4	0.00	0.00	0.00	0.02	0.02	0.04	0.64	0.01	0.00	0.00
H2	-	-	-	-	-	-	-	-	-	-
O2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-	-	-	-	0.00	0.00	0.00	0.00	-	0.00	0.00
HSO3-	-	-	-	0.00	0.00	0.00	0.00	-	0.00	0.00
HSO4-	-	-	-	0.56	0.56	0.55	0.27	-	0.01	0.01
H3O+	-	-	-	0.59	0.59	0.57	0.27	-	0.01	0.01
SO3-2	-	-	-	0.00	0.00	0.00	0.00	-	0.00	0.00
SO4-2	-	-	-	0.02	0.02	0.01	0.00	-	0.00	0.00
Mass Flow kg/sec										
H2O	0.00	0.00	0.00	8.91	8.91	9.43	8.04	5.91	5.66	5.63
H2SO4	0.00	0.00	0.00	2.03	2.02	4.21	63.12	1.23	0.09	0.01
H2	-	-	-	-	-	-	-	-	-	-
O2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO2	0.29	0.29	0.29	0.25	0.25	0.25	0.00	0.00	0.00	0.00
SO3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.08	0.00	0.00
OH-	-	-	-	0.00	0.00	0.00	0.00	-	0.00	0.00
HSO3-	-	-	-	0.00	0.00	0.00	0.00	-	0.00	0.00
HSO4-	-	-	-	54.69	54.72	53.20	25.90	-	1.22	1.23
H3O+	-	-	-	11.32	11.32	10.77	5.08	-	0.24	0.27
SO3-2	-	-	-	0.00	0.00	0.00	0.00	-	0.00	0.00
SO4-2	-	-	-	1.52	1.50	0.86	0.00	-	0.01	0.08
Total Flow kmol/sec	0.00	0.00	0.00	1.69	1.69	1.69	1.62	0.34	0.34	0.34
Total Flow kg/sec	0.30	0.30	0.30	78.71	78.71	78.71	102.13	7.23	7.23	7.23
Total Flow cum/sec	0.09	0.09	0.08	0.05	0.78	1.94	3.83	15.58	10.38	7.72

Table 51: Mass Balance for Case 3

Stream No	427	428	429	430	431	432	433	434	435	436
	FL-107	VL-106	FL-112	HX-124	HX-125	FL-110	MX-106	VL-107	HX-126	FL-113
	HX-123	FL-111	VL-106	FL-112	HX-124	HX-125	FL-110	FL-112	VL-107	HX-126
	LIQUID	LIQUID	MIXED	MISSING	MISSING	MISSING	LIQUID	LIQUID	MIXED	LIQUID
Substream: MIXED										
Temperature K	343.00	550.00	516.33				313.00	471.00	470.63	370.00
Pressure bar	1.00	1.00	0.30	0.30	0.30	0.30	0.30	0.30	0.10	0.10
Vapor Frac	-	-	0.06				-	-	0.00	-
Liquid Frac	1.00	1.00	0.94				1.00	1.00	1.00	1.00
Mole Flow kmol/sec										
H2O	0.31	0.27	0.29	-	-	-	0.00	0.22	0.22	0.16
H2SO4	0.00	0.78	0.80	-	-	-	0.00	0.73	0.73	0.67
H2	-	-	-	-	-	-	-	-	-	-
O2	0.00	0.00	0.00	-	-	-	0.00	0.00	0.00	0.00
SO2	0.00	0.00	0.00	-	-	-	0.00	0.00	0.00	0.00
SO3	0.00	0.00	0.00	-	-	-	0.00	0.00	0.00	0.00
OH-	0.00	0.00	0.00	-	-	-	0.00	0.00	0.00	0.00
HSO3-	0.00	0.00	0.00	-	-	-	0.00	0.00	0.00	0.00
HSO4-	0.01	0.12	0.10	-	-	-	0.00	0.16	0.16	0.23
H3O+	0.01	0.12	0.10	-	-	-	0.00	0.16	0.16	0.23
SO3-2	0.00	0.00	0.00	-	-	-	0.00	0.00	0.00	0.00
SO4-2	0.00	0.00	0.00	-	-	-	0.00	0.00	0.00	0.00
Mass Flow kg/sec										
H2O	5.63	4.80	5.17	-	-	-	0.00	4.00	4.01	2.89
H2SO4	0.00	76.26	78.18	-	-	-	0.00	71.89	71.93	65.85
H2	-	-	-	-	-	-	-	-	-	-
O2	0.00	0.00	0.00	-	-	-	0.00	0.00	0.00	0.00
SO2	0.00	0.00	0.00	-	-	-	0.00	0.00	0.00	0.00
SO3	0.00	0.00	0.03	-	-	-	0.00	0.00	0.00	0.00
OH-	0.00	0.00	0.00	-	-	-	0.00	0.00	0.00	0.00
HSO3-	0.00	0.00	0.00	-	-	-	0.00	0.00	0.00	0.00
HSO4-	1.22	11.57	9.64	-	-	-	0.00	15.90	15.86	21.87
H3O+	0.28	2.27	1.89	-	-	-	0.00	3.12	3.11	4.29
SO3-2	0.00	0.00	0.00	-	-	-	0.00	0.00	0.00	0.00
SO4-2	0.09	0.00	0.00	-	-	-	0.00	0.00	0.00	0.01
Total Flow kmol/sec	0.34	1.28	1.28	-	-	-	0.00	1.28	1.28	1.28
Total Flow kg/sec	7.23	94.91	94.91	-	-	-	0.00	94.91	94.91	94.91
Total Flow cum/sec	0.01	0.06	11.62	-	-	-	0.00	0.06	0.43	0.05

Table 52: Mass Balance for Case 3

Stream No	437	438	439	440	441	442	443	444	445	446
	PP-104	HX-127	FL-114	HX-128	FL-115	CO-104	MX-105	MX-105	HX-129	HX-130
	FL-113	PP-104	HX-127	FL-114	HX-128	FL-115	FL-114	FL-115	MX-105	HX-129
	LIQUID	LIQUID	MIXED	VAPOR	MIXED	VAPOR	LIQUID	LIQUID	MIXED	LIQUID
Substream: MIXED										
Temperature K	370.00	370.03	579.00	579.00	575.00	575.00	579.00	575.00	578.90	550.00
Pressure bar	0.10	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
Vapor Frac	-	-	0.46	1.00	0.97	1.00	-	-	0.00	-
Liquid Frac	1.00	1.00	0.54	-	0.03	-	1.00	1.00	1.00	1.00
Mole Flow kmol/sec										
H2O	0.49	0.49	1.47	1.19	1.18	1.17	0.28	0.01	0.29	0.27
H2SO4	0.52	0.52	1.41	0.15	0.16	0.12	1.27	0.03	1.30	1.28
H2	-	-	-	-	-	-	-	-	-	-
O2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO3	0.00	0.00	0.04	0.04	0.03	0.03	0.00	0.00	0.00	0.00
OH-	0.00	0.00	0.00	-	0.00	-	0.00	0.00	0.00	0.00
HSO3-	0.00	0.00	0.00	-	0.00	-	0.00	0.00	0.00	0.00
HSO4-	0.98	0.98	0.05	-	0.00	-	0.05	0.00	0.05	0.07
H3O+	0.99	0.99	0.05	-	0.00	-	0.05	0.00	0.05	0.07
SO3-2	0.00	0.00	0.00	-	0.00	-	0.00	0.00	0.00	0.00
SO4-2	0.00	0.00	0.00	-	0.00	-	0.00	0.00	0.00	0.00
Mass Flow kg/sec										
H2O	8.82	8.83	26.43	21.40	21.19	21.05	5.02	0.14	5.16	4.81
H2SO4	50.52	50.52	138.74	14.58	15.45	12.21	124.16	3.24	127.41	125.49
H2	-	-	-	-	-	-	-	-	-	-
O2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO2	0.08	0.08	0.08	0.08	0.08	0.08	0.00	0.00	0.00	0.00
SO3	0.00	0.00	2.96	2.93	2.11	2.11	0.03	0.00	0.03	0.01
OH-	0.00	0.00	0.00	-	0.00	-	0.00	0.00	0.00	0.00
HSO3-	0.00	0.00	0.00	-	0.00	-	0.00	0.00	0.00	0.00
HSO4-	94.94	94.93	4.38	-	0.14	-	4.38	0.14	4.51	6.42
H3O+	18.74	18.74	0.86	-	0.03	-	0.86	0.03	0.88	1.26
SO3-2	0.00	0.00	0.00	-	0.00	-	0.00	0.00	0.00	0.00
SO4-2	0.34	0.34	0.00	-	0.00	-	0.00	0.00	0.00	0.00
Total Flow kmol/sec	2.97	2.97	3.01	1.37	1.36	1.32	1.64	0.04	1.68	1.68
Total Flow kg/sec	173.44	173.44	173.44	38.99	38.99	35.44	134.45	3.55	137.99	137.99
Total Flow cum/sec	0.10	0.10	66.02	65.93	62.91	62.91	0.08	0.00	0.09	0.09

Table 53: Mass Balance for Case 3

Stream No	447	448	FEED-H2O
	PP-103	CO-103	MX-104
	FL-107	FL-113	
	LIQUID	VAPOR	LIQUID
Substream: MIXED			
Temperature K	343.00	370.00	373.15
Pressure bar	1.00	0.10	21.00
Vapor Frac	-	1.00	-
Liquid Frac	1.00	-	1.00
Mole Flow kmol/sec			
H2O	0.15	0.00	0.58
H2SO4	0.00	0.00	0.00
H2	-	-	-
O2	0.00	0.00	-
SO2	0.00	0.00	-
SO3	0.00	0.00	0.00
OH-	0.00	-	0.00
HSO3-	0.00	-	-
HSO4-	0.01	-	0.00
H3O+	0.02	-	0.00
SO3-2	0.00	-	-
SO4-2	0.00	-	0.00
Mass Flow kg/sec			
H2O	2.70	0.00	10.45
H2SO4	0.00	0.00	0.00
H2	-	-	-
O2	0.00	0.00	-
SO2	0.05	0.17	-
SO3	0.00	0.00	0.00
OH-	0.00	-	0.00
HSO3-	0.00	-	-
HSO4-	1.12	-	0.00
H3O+	0.30	-	0.00
SO3-2	0.00	-	-
SO4-2	0.20	-	0.00
Total Flow kmol/sec	0.18	0.00	0.58
Total Flow kg/sec	4.36	0.17	10.45
Total Flow cum/sec	0.00	0.87	0.01

Mass Balance: Case 4

Table 54: Mass Balance for Case 4

	101	102	103	104	105	106	107	108	109	110	111	112
Temperature K	712.1	744.9	812.1	579	610	651.3	708.1	823.1	943.1	1023.2	902.4	843.6
Pressure bar	1	1.5	3	3	3	3	3	3	3	3	3	3
Vapor Frac	1	1	1	0	0	1	1	1	1	1	1	1
Mole Flow kmol/sec	1.688	1.688	1.688	1.688	1.688	2.143	2.532	2.943	3.019	3.406	3.402	3.386
Mass Flow kg/sec	138.487	138.487	138.487	138.487	138.487	138.487	138.487	138.487	138.487	138.487	138.487	138.487
Volume Flow cum/sec	99.094	68.909	37.325	0.106	0.11	38.074	49.327	66.971	78.798	96.519	84.97	79.039
Mass Flow kg/sec												
SO3	0	0	0	0	0	36.502	67.593	100.547	106.604	47.23	46.86	45.612
SO2	0	0	0	0	0	0	0	0	0	48.207	48.207	48.207
O2	0	0	0	0	0	0	0	0	0	12.039	12.039	12.039
H2SO4	132.407	132.407	132.407	132.407	132.407	87.691	49.605	9.237	1.816	0.748	1.2	2.729
H2O	6.08	6.08	6.08	6.08	6.08	14.294	21.289	28.704	30.067	30.263	30.18	29.899
H2	0	0	0	0	0	0	0	0	0	0	0	0
Mole Flow kmol/sec												
SO3	0	0	0	0	0	0.456	0.844	1.256	1.331	0.59	0.585	0.57
SO2	0	0	0	0	0	0	0	0	0	0.752	0.752	0.752
O2	0	0	0	0	0	0	0	0	0	0.376	0.376	0.376
H2SO4	1.35	1.35	1.35	1.35	1.35	0.894	0.506	0.094	0.019	0.008	0.012	0.028
H2O	0.338	0.338	0.338	0.338	0.338	0.793	1.182	1.593	1.669	1.68	1.675	1.66
H2	0	0	0	0	0	0	0	0	0	0	0	0

Table 55: Mass Balance for Case 4

Stream No	201	202	203	204	205	206	207	208	209	210
	HX-104	HX-105	HX-106	HX-106	FL-101	FL-101	FL-101	CO-101	CO-101	HX-107
	CO-104	HX-104	HX-105	PP-103	HX-106	HX-136	HX-134	FL-101	FL-104	CO-101
	VAPOR	MIXED	MIXED	LIQUID	MIXED	MIXED	MIXED	VAPOR	VAPOR	VAPOR
Substream: MIXED										
Temperature K	752.75	613.15	573.15	343.14	393.15	393.00	393.00	393.15	506.00	751.07
Pressure bar	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00	21.00
Vapor Frac	1.00	0.90	0.76	-	0.31	0.12	1.00	1.00	1.00	1.00
Liquid Frac	-	0.10	0.24	1.00	0.69	0.88	0.00	-	-	-
Mole Flow kmol/sec										
H2O	1.18	2.34	2.16	0.00	1.49	0.17	0.00	0.18	1.03	1.20
H2SO4	0.13	0.65	0.66	0.00	0.02	0.00	0.00	0.00	0.00	0.00
H2	-	-	-	-	-	-	-	-	-	-
O2	0.00	0.38	0.38	0.00	0.38	0.00	0.00	0.38	0.00	0.38
SO2	0.00	0.75	0.75	0.00	0.75	0.01	0.01	0.75	0.01	0.77
SO3	0.03	0.10	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-	-	0.00	0.00	0.00	0.00	0.00	0.00	-	-	-
HSO3-	-	0.00	0.00	0.00	0.00	0.00	0.00	-	-	-
HSO4-	-	0.00	0.08	0.00	0.70	0.00	0.00	-	-	-
H3O+	-	0.00	0.08	0.00	0.75	0.00	0.00	-	-	-
SO3-2	-	0.00	0.00	0.00	0.00	0.00	0.00	-	-	-
SO4-2	-	0.00	0.00	0.00	0.02	0.00	0.00	-	-	-
Mass Flow kg/sec										
H2O	21.17	42.20	38.99	0.00	26.86	3.10	0.01	3.22	18.48	21.70
H2SO4	12.28	63.36	64.90	0.00	2.28	0.00	0.00	0.00	0.04	0.04
H2	-	-	-	-	-	-	-	-	-	-
O2	0.00	12.03	12.03	0.00	12.03	0.00	0.00	12.03	0.00	12.03
SO2	0.08	48.25	48.25	0.00	48.25	0.50	0.36	48.36	0.75	49.11
SO3	2.12	8.30	0.56	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-	-	0.00	0.00	0.00	0.00	0.00	0.00	-	-	-
HSO3-	-	0.00	0.00	0.00	0.00	0.00	0.00	-	-	-
HSO4-	-	0.00	7.87	0.00	68.42	0.00	0.00	-	-	-
H3O+	-	0.00	1.54	0.00	14.23	0.00	0.00	-	-	-
SO3-2	-	0.00	0.00	0.00	0.00	0.00	0.00	-	-	-
SO4-2	-	0.00	0.00	0.00	2.07	0.00	0.00	-	-	-
Total Flow kmol/sec	1.33	4.22	4.12	0.00	4.12	0.18	0.01	1.31	1.04	2.35
Total Flow kg/sec	35.64	174.14	174.14	0.01	174.15	3.60	0.38	63.61	19.27	82.88
Total Flow cum/sec	27.60	64.18	49.80	0.00	13.74	0.23	0.07	14.10	14.38	6.92

Table 56: Mass Balance for Case 4

Stream No	211	212	213	214	215	216	217	218	219	220
	HX-108	MX-101	MX-101	HX-109	FL-102	HX-110	FL-103	DR-101		TK-101
	HX-107	HX-108	FL-108	MX-101	HX-109	FL-102	HX-110	FL-103	DR-101	DR-101
	VAPOR	MIXED	VAPOR	MIXED	MIXED	VAPOR	MIXED	VAPOR	VAPOR	LIQUID
Substream: MIXED										
Temperature K	600.00	500.00	373.00	464.04	313.15	313.00	250.00	250.00	250.00	250.00
Pressure bar	21.00	21.00	21.00	21.00	21.00	21.00	21.00	21.00	21.00	21.00
Vapor Frac	1.00	1.00	1.00	1.00	0.18	1.00	0.70	1.00	1.00	-
Liquid Frac	-	0.00	-	0.00	0.82	-	0.30	-	-	1.00
Mole Flow kmol/sec										
H2O	1.20	1.20	0.05	1.25	1.18	0.00	0.00	0.00	-	0.00
H2SO4	0.00	0.00	0.00	0.00	0.00	0.00	-	-	-	-
H2	-	-	-	-	-	-	-	-	-	-
O2	0.38	0.38	0.00	0.38	0.38	0.38	0.38	0.38	0.38	-
SO2	0.77	0.77	0.75	1.52	1.48	0.19	0.18	0.02	-	0.02
SO3	0.00	0.00	0.00	0.00	0.00	0.00	-	-	-	-
OH-	-	0.00	-	0.00	0.00	-	0.00	-	-	0.00
HSO3-	-	0.00	-	0.00	0.03	-	0.00	-	-	0.00
HSO4-	-	0.00	-	0.00	0.00	-	-	-	-	-
H3O+	-	0.00	-	0.00	0.04	-	0.00	-	-	0.00
SO3-2	-	0.00	-	0.00	0.00	-	0.00	-	-	0.00
SO4-2	-	0.00	-	0.00	0.00	-	-	-	-	-
Mass Flow kg/sec										
H2O	21.70	21.69	0.83	22.52	21.27	0.05	0.03	0.00	-	0.00
H2SO4	0.04	0.00	0.00	0.00	0.00	0.00	-	-	-	-
H2	-	-	-	-	-	-	-	-	-	-
O2	12.03	12.03	0.06	12.09	12.09	12.04	12.04	12.03	12.03	-
SO2	49.11	49.11	48.06	97.17	94.96	11.90	11.85	1.06	-	1.06
SO3	0.00	0.00	0.00	0.00	0.00	0.00	-	-	-	-
OH-	-	0.00	-	0.00	0.00	-	0.00	-	-	0.00
HSO3-	-	0.00	-	0.00	2.79	-	0.06	-	-	0.00
HSO4-	-	0.03	-	0.04	0.00	-	-	-	-	-
H3O+	-	0.01	-	0.01	0.67	-	0.01	-	-	0.00
SO3-2	-	0.00	-	0.00	0.00	-	0.00	-	-	0.00
SO4-2	-	0.00	-	0.00	0.03	-	-	-	-	-
Total Flow kmol/sec	2.35	2.35	0.80	3.15	3.11	0.56	0.56	0.39	0.38	0.02
Total Flow kg/sec	82.88	82.88	48.95	131.83	131.83	23.99	23.99	13.09	12.03	1.06
Total Flow cum/sec	5.43	4.38	0.98	5.34	0.73	0.66	0.38	0.37	0.36	0.00

Table 57: Mass Balance for Case 4

Stream No	221	222	223	224	225	226	301	302	303	304
	TK-101	TK-101	HX-111	HX-112	FL-104	VL-104	EL-101	EL-101	EL-102	MX-102
	FL-103	FL-102	TK-101	FL-101	HX-112	FL-104	HX-111	MEM-101	EL-101	EL-102
	LIQUID	LIQUID	MIXED	LIQUID	MIXED	LIQUID	LIQUID	LIQUID	MIXED	VAPOR
Substream: MIXED										
Temperature K	250.00	313.00	309.37	393.15	506.00	506.00	373.15	373.15	373.15	373.15
Pressure bar	21.00	21.00	21.00	3.00	3.00	3.00	21.00	21.00	21.00	21.00
Vapor Frac	-	-	0.00	-	0.35	-	-	-	0.52	1.00
Liquid Frac	1.00	1.00	1.00	1.00	0.65	1.00	1.00	1.00	0.48	-
Mole Flow kmol/sec										
H2O	0.00	1.18	1.17	1.48	1.74	0.71	1.22	0.75	0.17	-
H2SO4	-	0.00	0.00	0.02	0.25	0.25	0.00	-	0.42	-
H2	-	-	-	-	-	-	-	-	0.75	0.75
O2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00	-
SO2	0.17	1.30	1.48	0.01	0.01	0.00	1.50	-	0.76	-
SO3	-	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00	-
OH-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-
HSO3-	0.00	0.03	0.04	0.00	0.00	0.00	0.01	-	0.00	-
HSO4-	-	0.00	0.00	0.71	0.50	0.50	0.00	-	0.33	-
H3O+	0.00	0.04	0.04	0.75	0.50	0.50	0.01	0.00	0.33	-
SO3-2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00	-
SO4-2	-	0.00	0.00	0.02	0.00	0.00	0.00	-	0.00	-
Mass Flow kg/sec										
H2O	0.03	21.22	21.08	26.63	31.27	12.83	22.06	13.55	3.03	-
H2SO4	-	0.00	0.00	1.91	24.78	24.80	0.00	-	41.46	-
H2	-	-	-	-	-	-	-	-	1.52	1.52
O2	0.01	0.05	0.06	0.00	0.00	0.00	0.06	-	0.06	-
SO2	10.79	83.06	94.62	0.75	0.75	0.00	96.35	-	48.99	-
SO3	-	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00	-
OH-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-
HSO3-	0.06	2.80	3.22	0.00	0.00	0.00	1.03	-	0.00	-
HSO4-	-	0.00	0.00	68.50	48.24	48.36	0.02	-	31.90	-
H3O+	0.01	0.67	0.77	14.36	9.46	9.48	0.25	0.00	6.29	-
SO3-2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	0.00	-
SO4-2	-	0.03	0.03	2.37	0.01	0.01	0.02	-	0.09	-
Total Flow kmol/sec	0.17	2.55	2.73	2.99	2.99	1.96	2.76	0.75	2.77	0.75
Total Flow kg/sec	10.90	107.84	119.79	114.52	114.52	95.49	119.79	13.55	133.34	1.52
Total Flow cum/sec	0.01	0.07	0.08	0.08	14.46	0.08	0.09	0.01	2.13	1.12

Table 58: Mass Balance for Case 4

Stream No	305	306	307	308	309	310	311	312	313	314
	MX-102	HX-113	FL-105	HX-114	DR-102		MX-103	MX-103	HX-115	MX-104
	MEM-101	MX-102	HX-113	FL-105	HX-114	DR-102	DR-102	FL-105	MX-103	HX-115
	LIQUID	MIXED	MIXED	VAPOR	MIXED	VAPOR	LIQUID	LIQUID	LIQUID	LIQUID
Substream: MIXED										
Temperature K	373.15	348.61	348.15	348.15	313.15	313.15	313.15	348.15	335.45	373.15
Pressure bar	21.00	21.00	21.00	21.00	20.00	20.00	20.00	21.00	20.00	21.00
Vapor Frac	-	0.97	0.97	1.00	0.98	1.00	-	-	-	-
Liquid Frac	1.00	0.03	0.03	-	0.02	-	1.00	1.00	1.00	1.00
Mole Flow kmol/sec										
H2O	0.04	0.04	0.04	0.01	0.01	-	0.01	0.03	0.04	0.04
H2SO4	0.00	0.00	0.00	0.00	-	-	-	0.00	0.00	0.00
H2	0.00	0.75	0.75	0.75	0.75	0.75	-	0.00	0.00	0.00
O2	-	-	-	-	-	-	-	-	-	-
SO2	-	-	-	-	-	-	-	-	-	-
SO3	0.00	0.00	0.00	0.00	-	-	-	0.00	0.00	0.00
OH-	0.00	0.00	0.00	-	0.00	-	0.00	0.00	0.00	0.00
HSO3-	-	-	-	-	-	-	-	-	-	-
HSO4-	0.00	0.00	0.00	-	-	-	-	0.00	0.00	0.00
H3O+	0.00	0.00	0.00	-	0.00	-	0.00	0.00	0.00	0.00
SO3-2	-	-	-	-	-	-	-	-	-	-
SO4-2	0.00	0.00	0.00	-	-	-	-	0.00	0.00	0.00
Mass Flow kg/sec										
H2O	0.71	0.71	0.71	0.26	0.26	-	0.26	0.45	0.71	0.71
H2SO4	0.00	0.00	0.00	0.00	-	-	-	0.00	0.00	0.00
H2	0.00	1.52	1.52	1.52	1.52	1.52	-	0.00	0.00	0.00
O2	-	-	-	-	-	-	-	-	-	-
SO2	-	-	-	-	-	-	-	-	-	-
SO3	0.00	0.00	0.00	0.00	-	-	-	0.00	0.00	0.00
OH-	0.00	0.00	0.00	-	0.00	-	0.00	0.00	0.00	0.00
HSO3-	-	-	-	-	-	-	-	-	-	-
HSO4-	0.00	0.00	0.00	-	-	-	-	0.00	0.00	0.00
H3O+	0.00	0.00	0.00	-	0.00	-	0.00	0.00	0.00	0.00
SO3-2	-	-	-	-	-	-	-	-	-	-
SO4-2	0.00	0.00	0.00	-	-	-	-	0.00	0.00	0.00
Total Flow kmol/sec	0.04	0.79	0.79	0.77	0.77	0.75	0.01	0.03	0.04	0.04
Total Flow kg/sec	0.71	2.23	2.23	1.78	1.78	1.52	0.26	0.45	0.71	0.71
Total Flow cum/sec	0.00	1.07	1.07	1.07	1.00	0.99	0.00	0.00	0.00	0.00

Table 59: Mass Balance for Case 4

Stream No	315	316	317	401	402	403	404	405	406	407
	MEM-101	VL-101	HX-116	FL-106	HX-117	FL-107	CO-102	HX-118	FL-108	MX-106
	MX-104	EL-102	VL-101	HX-116	FL-106	HX-117	FL-107	CO-102	HX-118	FL-108
	LIQUID	MIXED	MIXED	MIXED	VAPOR	MIXED	VAPOR	VAPOR	MIXED	LIQUID
Substream: MIXED										
Temperature K	373.15	373.15	266.85	365.00	365.00	343.00	343.00	708.67	373.00	373.00
Pressure bar	21.00	21.00	1.00	1.00	1.00	1.00	1.00	21.00	21.00	21.00
Vapor Frac	-	0.00	0.30	0.38	1.00	1.00	1.00	1.00	0.91	-
Liquid Frac	1.00	1.00	0.70	0.62	-	0.00	-	-	0.09	1.00
Mole Flow kmol/sec										
H2O	0.79	0.10	0.06	0.17	0.00	0.00	0.11	0.11	0.11	0.07
H2SO4	0.00	0.35	0.32	0.43	0.00	0.00	0.00	0.00	0.00	0.00
H2	0.00	-	-	-	-	-	-	-	-	-
O2	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO2	-	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.76	0.01
SO3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-	0.00	0.00	0.00	0.00	-	0.00	-	-	0.00	0.00
HSO3-	-	0.00	0.00	0.00	-	0.00	-	-	0.00	0.00
HSO4-	0.00	0.39	0.43	0.32	-	0.00	-	-	0.00	0.00
H3O+	0.00	0.40	0.43	0.32	-	0.00	-	-	0.00	0.00
SO3-2	-	0.00	0.00	0.00	-	0.00	-	-	0.00	0.00
SO4-2	0.00	0.01	0.00	0.00	-	0.00	-	-	0.00	0.00
Mass Flow kg/sec										
H2O	14.26	1.77	1.13	3.11	0.02	0.02	2.06	2.06	2.06	1.23
H2SO4	0.00	34.46	31.74	42.54	0.00	0.00	0.00	0.00	0.00	0.00
H2	0.00	-	-	-	-	-	-	-	-	-
O2	-	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.06	0.00
SO2	-	48.99	48.99	48.99	48.53	48.53	48.53	48.53	48.52	0.46
SO3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-	0.00	0.00	0.00	0.00	-	0.00	-	-	0.00	0.00
HSO3-	-	0.00	0.00	0.00	-	0.00	-	-	0.02	0.02
HSO4-	0.00	37.91	41.56	30.86	-	0.00	-	-	0.00	0.00
H3O+	0.00	7.60	8.16	6.07	-	0.00	-	-	0.00	0.00
SO3-2	-	0.00	0.00	0.00	-	0.00	-	-	0.00	0.00
SO4-2	0.00	1.01	0.04	0.06	-	0.00	-	-	0.00	0.00
Total Flow kmol/sec	0.79	2.02	2.01	2.01	0.76	0.76	0.87	0.87	0.87	0.08
Total Flow kg/sec	14.26	131.79	131.69	131.69	48.61	48.61	50.66	50.66	50.66	1.71
Total Flow cum/sec	0.01	0.09	13.29	22.97	22.92	21.50	24.68	2.43	0.98	0.00

Table 60: Mass Balance for Case 4

Stream No	408	409	410	411	412	413	414	415	416	417
	PP-105	HX-135	HX-136	VL-102	FL-109	HX-119	FL-110	CO-103	HX-131	HX-132
	MX-106	PP-105	HX-135	FL-106	VL-102	FL-109	HX-119	FL-110	CO-103	HX-131
	MIXED	MIXED	MIXED	LIQUID	MIXED	VAPOR	MIXED	VAPOR	VAPOR	VAPOR
Substream: MIXED										
Temperature K	317.89	351.10	350.00	365.00	364.25	325.00	313.00	313.00	769.74	685.00
Pressure bar	0.30	3.00	3.00	1.00	0.30	0.30	0.30	0.30	3.00	3.00
Vapor Frac	0.06	0.03	0.03	-	0.00	1.00	1.00	1.00	1.00	1.00
Liquid Frac	0.94	0.97	0.97	1.00	1.00	-	0.00	-	-	-
Mole Flow kmol/sec										
H2O	0.17	0.17	0.17	0.17	0.17	0.00	0.00	0.00	0.00	0.00
H2SO4	0.00	0.00	0.00	0.43	0.43	0.00	0.00	0.00	0.00	0.00
H2	-	-	-	-	-	-	-	-	-	-
O2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO2	0.01	0.01	0.01	0.01	0.01	0.00	0.00	0.00	0.01	0.01
SO3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-	0.00	0.00	0.00	0.00	0.00	-	0.00	-	-	-
HSO3-	0.00	0.00	0.00	0.00	0.00	-	0.00	-	-	-
HSO4-	0.00	0.00	0.00	0.32	0.32	-	0.00	-	-	-
H3O+	0.00	0.00	0.00	0.32	0.32	-	0.00	-	-	-
SO3-2	0.00	0.00	0.00	0.00	0.00	-	0.00	-	-	-
SO4-2	0.00	0.00	0.00	0.00	0.00	-	0.00	-	-	-
Mass Flow kg/sec										
H2O	3.10	3.09	3.09	3.08	3.09	0.00	0.00	0.01	0.01	0.01
H2SO4	0.00	0.00	0.00	42.54	42.56	0.00	0.00	0.00	0.00	0.00
H2	-	-	-	-	-	-	-	-	-	-
O2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO2	0.49	0.49	0.48	0.46	0.46	0.14	0.14	0.12	0.36	0.36
SO3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-	0.00	0.00	0.00	0.00	0.00	-	0.00	-	-	-
HSO3-	0.01	0.02	0.02	0.00	0.00	-	0.00	-	-	-
HSO4-	0.00	0.00	0.00	30.86	30.84	-	0.00	-	-	-
H3O+	0.00	0.00	0.00	6.07	6.07	-	0.00	-	-	-
SO3-2	0.00	0.00	0.00	0.00	0.00	-	0.00	-	-	-
SO4-2	0.00	0.00	0.00	0.06	0.06	-	0.00	-	-	-
Total Flow kmol/sec	0.18	0.18	0.18	1.25	1.25	0.00	0.00	0.00	0.01	0.01
Total Flow kg/sec	3.60	3.60	3.60	83.08	83.08	0.14	0.14	0.13	0.38	0.38
Total Flow cum/sec	0.94	0.06	0.06	0.05	0.56	0.20	0.19	0.21	0.14	0.12

Table 61: Mass Balance for Case 4

Stream No	418	419	420	421	422	423	424	425	426	427
	HX-133	HX-134	VL-103	HX-120	FL-113	FL-111	HX-121	HX-122	HX-123	FL-107
	HX-132	HX-133	FL-109	VL-103	HX-120	VL-104	FL-111	HX-121	HX-122	HX-123
	VAPOR	VAPOR	LIQUID	MIXED	MIXED	MIXED	VAPOR	MIXED	MIXED	LIQUID
Substream: MIXED										
Temperature K	645.00	600.00	325.00	324.58	370.00	472.80	472.00	430.00	390.00	343.00
Pressure bar	3.00	3.00	0.30	0.10	0.10	1.00	1.00	1.00	1.00	1.00
Vapor Frac	1.00	1.00	-	0.00	0.00	0.06	1.00	1.00	1.00	-
Liquid Frac	-	-	1.00	1.00	1.00	0.94	-	0.00	0.00	1.00
Mole Flow kmol/sec										
H2O	0.00	0.00	0.13	0.13	0.18	0.71	0.11	0.11	0.11	0.11
H2SO4	0.00	0.00	0.40	0.40	0.44	0.25	0.00	0.00	0.00	0.00
H2	-	-	-	-	-	-	-	-	-	-
O2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO2	0.01	0.01	0.01	0.01	0.01	0.00	0.00	0.00	0.00	0.00
SO3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-	-	-	0.00	0.00	0.00	0.00	-	0.00	0.00	0.00
HSO3-	-	-	0.00	0.00	0.00	0.00	-	0.00	0.00	0.00
HSO4-	-	-	0.36	0.36	0.31	0.50	-	0.00	0.00	0.00
H3O+	-	-	0.36	0.36	0.31	0.50	-	0.00	0.00	0.00
SO3-2	-	-	0.00	0.00	0.00	0.00	-	0.00	0.00	0.00
SO4-2	-	-	0.00	0.00	0.00	0.00	-	0.00	0.00	0.00
Mass Flow kg/sec										
H2O	0.01	0.01	2.39	2.39	3.19	12.77	2.04	2.04	2.04	2.04
H2SO4	0.00	0.00	38.77	38.78	43.13	24.49	0.00	0.00	0.00	0.00
H2	-	-	-	-	-	-	-	-	-	-
O2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO2	0.36	0.36	0.32	0.32	0.32	0.00	0.00	0.00	0.00	0.00
SO3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-	-	-	0.00	0.00	0.00	0.00	-	0.00	0.00	0.00
HSO3-	-	-	0.00	0.00	0.00	0.00	-	0.00	0.00	0.00
HSO4-	-	-	34.58	34.56	30.28	48.67	-	0.00	0.00	0.00
H3O+	-	-	6.81	6.80	5.96	9.54	-	0.00	0.00	0.00
SO3-2	-	-	0.00	0.00	0.00	0.00	-	0.00	0.00	0.00
SO4-2	-	-	0.08	0.08	0.05	0.02	-	0.00	0.00	0.00
Total Flow kmol/sec	0.01	0.01	1.25	1.25	1.25	1.96	0.11	0.11	0.11	0.11
Total Flow kg/sec	0.38	0.38	82.94	82.94	82.94	95.49	2.05	2.05	2.05	2.05
Total Flow cum/sec	0.12	0.11	0.05	0.96	1.44	4.98	4.43	4.02	3.63	0.00

Table 62: Mass Balance for Case 4

Stream No	428	429	430	431	432	433	434	435	436	437
	PP-103	VL-105	FL-112	HX-124	HX-125	FL-110	MX-106	VL-106	HX-126	FL-113
	FL-107	FL-111	VL-105	FL-112	HX-124	HX-125	FL-110	FL-112	VL-106	HX-126
	LIQUID	LIQUID	MIXED	VAPOR	MIXED	LIQUID	LIQUID	LIQUID	MIXED	LIQUID
Substream: MIXED										
Temperature K	343.00	472.00	441.75	441.00	390.00	313.00	313.00	441.00	417.48	370.00
Pressure bar	1.00	1.00	0.30	0.30	0.30	0.30	0.30	0.30	0.10	0.10
Vapor Frac	-	-	0.06	1.00	1.00	-	-	-	0.05	-
Liquid Frac	1.00	1.00	0.94	-	0.00	1.00	1.00	1.00	0.95	1.00
Mole Flow kmol/sec										
H2O	0.00	0.59	0.59	0.10	0.10	0.10	0.10	0.48	0.48	0.37
H2SO4	0.00	0.24	0.24	0.00	0.00	0.00	0.00	0.24	0.24	0.13
H2	-	-	-	-	-	-	-	-	-	-
O2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-	0.00	0.00	0.00	-	0.00	0.00	0.00	0.00	0.00	0.00
HSO3-	0.00	0.00	0.00	-	0.00	0.00	0.00	0.00	0.00	0.00
HSO4-	0.00	0.51	0.51	-	0.00	0.00	0.00	0.51	0.51	0.61
H3O+	0.00	0.51	0.51	-	0.00	0.00	0.00	0.51	0.51	0.62
SO3-2	0.00	0.00	0.00	-	0.00	0.00	0.00	0.00	0.00	0.00
SO4-2	0.00	0.00	0.00	-	0.00	0.00	0.00	0.00	0.00	0.00
Mass Flow kg/sec										
H2O	0.00	10.63	10.63	1.88	1.88	1.88	1.86	8.65	8.65	6.67
H2SO4	0.00	23.99	24.01	0.00	0.00	0.00	0.00	23.47	23.48	13.00
H2	-	-	-	-	-	-	-	-	-	-
O2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SO2	0.00	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.00	0.00
SO3	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OH-	0.00	0.00	0.00	-	0.00	0.00	0.00	0.00	0.00	0.00
HSO3-	0.00	0.00	0.00	-	0.00	0.00	0.01	0.00	0.00	0.00
HSO4-	0.00	49.15	49.10	-	0.00	0.00	0.00	49.63	49.58	59.67
H3O+	0.00	9.64	9.64	-	0.00	0.00	0.00	9.75	9.75	11.84
SO3-2	0.00	0.00	0.00	-	0.00	0.00	0.00	0.00	0.00	0.00
SO4-2	0.00	0.02	0.05	-	0.00	0.00	0.00	0.05	0.09	0.38
Total Flow kmol/sec	0.00	1.85	1.85	0.10	0.10	0.10	0.10	1.74	1.74	1.74
Total Flow kg/sec	0.01	93.44	93.44	1.88	1.88	1.88	1.90	91.55	91.55	91.55
Total Flow cum/sec	0.00	0.07	14.18	12.72	11.23	0.00	0.00	0.06	29.02	0.06

Table 63: Mass Balance for Case 4

Stream No	439	440	441	442	443	444	445	446	447	448	449	FEED-H2O
	CO-103	PP-104	HX-127	FL-114	MX-105	HX-128	FL-115	CO-104	MX-105	HX-129	HX-130	MX-104
	FL-113	FL-113	PP-104	HX-127	FL-114	FL-114	HX-128	FL-115	FL-115	MX-105	HX-129	
	VAPOR	LIQUID	LIQUID	MIXED	LIQUID	VAPOR	MIXED	VAPOR	LIQUID	MIXED	LIQUID	LIQUID
Substream: MIXED												
Temperature K	370.00	370.00	370.03	579.00	579.00	579.00	575.00	575.00	575.00	578.90	550.00	373.15
Pressure bar	0.10	0.10	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	21.00
Vapor Frac	1.00	-	-	0.46	-	1.00	0.97	1.00	-	0.00	-	-
Liquid Frac	-	1.00	1.00	0.54	1.00	-	0.03	-	1.00	1.00	1.00	1.00
Mole Flow kmol/sec												
H2O	0.00	0.49	0.49	1.47	0.28	1.19	1.18	1.18	0.01	0.29	0.27	0.75
H2SO4	0.00	0.52	0.52	1.42	1.27	0.15	0.16	0.13	0.03	1.30	1.29	0.00
H2	-	-	-	-	-	-	-	-	-	-	-	-
O2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	-	-
SO2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-
SO3	0.00	0.00	0.00	0.04	0.00	0.04	0.03	0.03	0.00	0.00	0.00	0.00
OH-	-	0.00	0.00	0.00	0.00	-	0.00	-	0.00	0.00	0.00	0.00
HSO3-	-	0.00	0.00	0.00	0.00	-	0.00	-	0.00	0.00	0.00	-
HSO4-	-	0.98	0.98	0.05	0.05	-	0.00	-	0.00	0.05	0.07	0.00
H3O+	-	0.99	0.99	0.05	0.05	-	0.00	-	0.00	0.05	0.07	0.00
SO3-2	-	0.00	0.00	0.00	0.00	-	0.00	-	0.00	0.00	0.00	-
SO4-2	-	0.00	0.00	0.00	0.00	-	0.00	-	0.00	0.00	0.00	0.00
Mass Flow kg/sec												
H2O	0.00	8.87	8.87	26.57	5.05	21.52	21.31	21.17	0.14	5.19	4.83	13.55
H2SO4	0.00	50.67	50.68	139.37	124.70	14.66	15.54	12.28	3.26	127.97	126.04	0.00
H2	-	-	-	-	-	-	-	-	-	-	-	-
O2	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	-	-
SO2	0.25	0.08	0.08	0.08	0.00	0.08	0.08	0.08	0.00	0.00	0.00	-
SO3	0.00	0.00	0.00	2.98	0.03	2.95	2.12	2.12	0.00	0.03	0.01	0.00
OH-	-	0.00	0.00	0.00	0.00	-	0.00	-	0.00	0.00	0.00	0.00
HSO3-	-	0.00	0.00	0.00	0.00	-	0.00	-	0.00	0.00	0.00	-
HSO4-	-	95.44	95.43	4.40	4.40	-	0.14	-	0.14	4.53	6.45	0.00
H3O+	-	18.84	18.84	0.86	0.86	-	0.03	-	0.03	0.89	1.26	0.00
SO3-2	-	0.00	0.00	0.00	0.00	-	0.00	-	0.00	0.00	0.00	-
SO4-2	-	0.35	0.35	0.00	0.00	-	0.00	-	0.00	0.00	0.00	0.00
Total Flow kmol/sec	0.00	2.99	2.99	3.02	1.64	1.38	1.37	1.33	0.04	1.69	1.69	0.75
Total Flow kg/sec	0.25	174.24	174.24	174.24	135.03	39.21	39.21	35.64	3.57	138.60	138.60	13.55
Total Flow cum/sec	1.26	0.10	0.10	66.39	0.09	66.30	63.26	63.26	0.00	0.09	0.09	0.01

10. Appendix C: Decomposer Section Mass balance

Detail mass balance of the decomposition section: Case 1

Table 64: Decomposition Section Detail Mass balance

HX-103		
IN		
m_{in}	1687.5	mol/s
$mass_{in}$	138.4	kg/s
m_{H2SO4}	1350.0	mol/s
m_{H2SO4}	0.8	mol
Cp_{H2SO4}	117.5	J/mol K
m_{H2O}	337.5	mol/s
m_{H2O}	0.2	mol
Cp_{H2O}	36.7	J/mol K
Tin	610.0	K
UIT		
m_{uit}	2431.2	mol/s
$mass_{uit}$	138.4	kg/s
m_{SO3}	743.7	mol/s
m_{SO3}	0.3	mol %
m_{SO3}	59.5	kg/s
m_{H2O}	1081.2	mol/s
m_{H2O}	0.4	mol %
m_{H2O}	19.5	kg/s
m_{H2SO4}	606.3	mol/s
m_{H2SO4}	0.2	mol %
m_{H2SO4}	59.4	kg/s
Vapour	1.0	frac
Liquid	0.0	frac
Tuit	651.3	K
$\mathbf{T_{Cp}}$	0.6	
ΔT	-41.3	K
Q	7065161.1	Watt
Q	7.1	MWt
Qvap	84.2	MWt
Qreaction	72.5	MWt
Q_{TOT}	163.8	MWt

Table 65: Decomposition Section Detail Mass balance

EX-101 (RECOUP-1)

Product stream side		
IN		
m_{in}	2431.2	mol/s
$mass_{in}$	138.4	kg/s
m_{H2SO4}	606.3	mol/s
m_{H2SO4}	0.2	mol %
Cp_{H2SO4}	120.2	J/mol K
m_{H2O}	1081.2	mol/s
m_{H2O}	0.4	mol %
Cp_{H2O}	37.2	J/mol K
m_{SO3}	743.7	mol/s
m_{SO3}	0.3	mol %
Cp_{SO3}	69.7	J/mol K
Vap frac	1.0	frac
Liq frac	0.0	frac
Tin	651.0	K
UIT		
m_{uit}	2736.1	mol/s
$mass_{uit}$	138.4	kg/s
m_{H2SO4}	301.4	mol/s
m_{H2SO4}	0.1	mol %
m_{H2SO4}	29.5	kg/s
m_{H2O}	1386.1	mol/s
m_{H2O}	0.5	mol %
m_{H2O}	25.0	kg/s
m_{SO3}	1048.6	mol/s
m_{SO3}	0.4	mol %
m_{SO3}	84.0	kg/s
Vap frac	1.0	frac
Liq frac	0.0	frac
Tuit	701.0	K
$\mathbf{T_{Cp}}$	0.7	
ΔT	-50.0	K
Q	8247855.0	Watt
Q	8.2	MWt
Qvap	0.0	MWt
Qreaction	29.7	
Q_{TOT}	37.0	MWt

Heater stream side		
IN		
m_{in}	3519.8	mol/s
$mass_{in}$	138.4	kg/s
m_{SO3}	379.7	mol/s
m_{SO3}	0.1	mol %
Cp_{SO3}	73.9	J/mol K
m_{H2SO4}	1.8	mol/s
m_{H2SO4}	0.0	mol %
Cp_{H2SO4}	128.3	J/mol K
m_{SO2}	968.4	mol/s
m_{SO2}	0.3	mol %
Cp_{SO2}	53.2	J/mol K
m_{O2}	484.2	mol/s
m_{O2}	0.1	mol %
Cp_{O2}	33.8	J/mol K
m_{H2O}	1685.6	mol/s
m_{H2O}	0.5	mol %
Cp_{H2O}	39.5	J/mol K
Tin	960.0	K
UIT		
m_{uit}	3519.8	mol/s
$mass_{uit}$	138.4	kg/s
m_{SO3}	351.9	mol/s
m_{SO3}	0.1	mol %
Cp_{SO3}	73.9	J/mol K
m_{H2SO4}	29.6	mol/s
m_{H2SO4}	0.0	mol %
Cp_{H2SO4}	128.3	J/mol K
m_{SO2}	968.4	mol/s
m_{SO2}	0.3	mol %
Cp_{SO2}	53.2	J/mol K
m_{O2}	484.2	mol/s
m_{O2}	0.1	mol %
Cp_{O2}	33.8	J/mol K
m_{H2O}	1657.8	mol/s
m_{H2O}	0.5	mol %
Cp_{H2O}	39.5	J/mol K
Tuit	759.0	K
$\mathbf{T_{Cp}}$	0.9	
ΔT	201.0	K
Q	32710296.3	Watt
Qreaction	2.8	MWt
Q	35.5	MWt

Table 66: Decomposition Section Detail Mass balance

RX-101 (H2SO4 REACTOR)		
IN		
m_{in}	2736.1	mol/s
$mass_{in}$	138.4	kg/s
m_{H2SO4}	301.4	mol/s
m_{H2SO4}	0.1	mol
Cp_{H2SO4}	124.4	J/mol K
m_{H2O}	1386.1	mol/s
m_{H2O}	0.5	mol
Cp_{H2O}	38.3	J/mol K
m_{SO3}	1048.6	mol/s
m_{SO3}	0.4	mol %
Cp_{SO3}	38.3	J/mol K
Tin	701.0	K
UIT		
m_{uit}	3019.4	mol/s
$mass_{uit}$	138.5	kg/s
m_{SO3}	1331.9	mol/s
m_{SO3}	0.4	mol %
m_{SO3}	106.6	kg/s
m_{H2O}	1669.4	mol/s
m_{H2O}	0.6	mol %
m_{H2O}	30.0	kg/s
m_{H2SO4}	18.1	mol/s
m_{H2SO4}	0.0	mol %
m_{H2SO4}	1.8	kg/s
Tuit	823.2	K
$\mathbf{T_{Cp}}$	0.8	
ΔT	-122.2	K
Q	11059940.4	Watt
Q	11.1	MWt
Qreaction	27.6	MWt
Qvap	0.0	MWt
Q_{TOT}	38.7	MWt
Conversion	1.0	

Table 67: Decomposition Section Detail Mass balance

EX-102 (RECOUP-2)						
Product stream side				**Heater stream side**		
IN				**IN**		
m_{in}	3019.4	mol/s		m_{in}	3516.7	mol/s
$mass_{in}$	138.5	kg/s		$mass_{in}$	138.4	kg/s
m_{H2SO4}	18.1	mol/s		m_{SO3}	376.6	mol/s
m_{H2SO4}	0.0	mol %		m_{SO3}	0.1	mol %
Cp_{H2SO4}	130.0	J/mol K		Cp_{SO3}	76.5	J/mol K
m_{H2O}	1669.4	mol/s		m_{H2SO4}	5.0	mol/s
m_{H2O}	0.6	mol %		m_{H2SO4}	0.0	mol %
Cp_{H2O}	40.1	J/mol K		Cp_{H2SO4}	134.0	J/mol K
m_{SO3}	1331.9	mol/s		m_{SO2}	968.4	mol/s
m_{SO3}	0.4	mol %		m_{SO2}	0.3	mol %
Cp_{SO3}	74.8	J/mol K		Cp_{SO2}	54.9	J/mol K
Vap frac	1.0	frac		m_{O2}	484.2	mol/s
Liq frac	0.0	frac		m_{O2}	0.1	mol %
Tin	823.2	K		Cp_{O2}	34.7	J/mol K
UIT				m_{H2O}	1682.5	mol/s
m_{uit}	1687.5	mol/s		m_{H2O}	0.5	mol %
$mass_{uit}$	138.5	kg/s		Cp_{H2O}	41.9	J/mol K
m_{H2SO4}	5.0	mol/s		**Tin**	1143.2	K
m_{H2SO4}	0.0	mol %		**UIT**		
m_{H2SO4}	0.5	kg/s		m_{uit}	3516.7	mol/s
m_{H2O}	1682.5	mol/s		$mass_{uit}$	138.4	kg/s
m_{H2O}	0.6	mol %		m_{SO3}	379.7	mol/s
m_{H2O}	30.3	kg/s		m_{SO3}	0.1	mol %
m_{SO3}	1345.0	mol/s		Cp_{SO3}	76.5	J/mol K
m_{SO3}	0.4	mol %		m_{H2SO4}	1.8	mol/s
m_{SO3}	107.7	kg/s		m_{H2SO4}	0.0	mol %
Vap frac	1.0	frac		Cp_{H2SO4}	134.0	J/mol K
Liq frac	0.0	frac		m_{SO2}	968.4	mol/s
Tuit	999.2	K		m_{SO2}	0.3	mol %
T_{Cp}	0.9			Cp_{SO2}	54.9	J/mol K
ΔT	-176.1	K		m_{O2}	484.2	mol/s
Q	29749294.5	Watt		m_{O2}	0.1	mol %
Q	29.7	MWt		Cp_{O2}	34.7	J/mol K
Qvap	0.0	MWt		m_{H2O}	1685.6	mol/s
Qreaction	0.0			m_{H2O}	0.5	mol %
Q_{TOT}	29.7	MWt		Cp_{H2O}	41.9	J/mol K
				Tuit	960.0	K
				T_{Cp}	1.1	
				ΔT	183.2	K
				Q	31123131.3	Watt
				Qreaction	0.3	MWt

Table 68: Decomposition Section Detail Mass balance

RX-102 (SO3 REACTOR)		
IN		
m_{in}	3032.5	mol/s
$mass_{in}$	138.4	kg/s
m_{SO3}	1345.0	mol/s
m_{SO3}	0.4	mol %
Cp_{SO3}	76.7	J/mol K
m_{H2O}	1682.5	mol/s
m_{H2O}	0.6	mol %
Cp_{H2O}	42.2	J/mol K
m_{H2SO4}	5.0	mol/s
m_{H2SO4}	0.0	mol %
Cp_{H2SO4}	134.5	J/mol K
Tin	999.2	K
UIT		
m_{uit}	3516.7	mol/s
$mass_{uit}$	138.4	kg/s
m_{SO3}	376.6	mol/s
m_{SO3}	0.1	mol %
m_{SO3}	30.2	kg/s
m_{H2O}	1682.5	mol/s
m_{H2O}	0.5	mol %
m_{H2O}	30.3	kg/s
m_{O2}	484.2	mol/s
m_{O2}	0.1	mol %
m_{O2}	15.5	kg/s
m_{SO2}	968.4	mol/s
m_{SO2}	0.3	mol %
m_{SO2}	62.0	kg/s
m_{H2SO4}	5.0	mol/s
m_{H2SO4}	0.0	mol %
m_{H2SO4}	0.5	kg/s
Tuit	1143.2	K
T_{Cp}	1.1	
ΔT	-143.9	K
Q	25156242.0	Watt
Qheating	25.2	MWt
Q	95793603.7	Watt
Qreaction	95.8	MWt
Q_{TOT}	120.9	MWt
Conversion	0.7	

Detail mass balance of the decomposition section: Case 2

Table 69: Decomposition mass balance - Case 2

HX-103		
IN		
m_{in}	1687.5	mol/s
$mass_{in}$	138.4	kg/s
m_{H2SO4}	1350.0	mol/s
m_{H2SO4}	0.8	mol
Cp_{H2SO4}	121.1	J/mol K
m_{H2O}	337.5	mol/s
m_{H2O}	0.2	mol
Cp_{H2O}	37.4	J/mol K
Tin	610.0	K
UIT		
m_{uit}	2119.0	mol/s
$mass_{uit}$	138.4	kg/s
m_{SO3}	431.0	mol/s
m_{SO3}	0.2	mol %
m_{SO3}	34.5	kg/s
m_{H2O}	769.0	mol/s
m_{H2O}	0.4	mol %
m_{H2O}	13.8	kg/s
m_{H2SO4}	919.0	mol/s
m_{H2SO4}	0.4	mol %
m_{H2SO4}	90.1	kg/s
Vapour	1.0	frac
Liquid	0.0	frac
Tuit	775.0	K
T_{Cp}	0.7	
ΔT	-165.0	K
Q	29054264.2	Watt
Q	29.1	MWt
Qvap	84.2	MWt
Qreaction	42.0	MWt
Q_{TOT}	155.3	MWt

Table 70: Decomposition mass balance - Case 2

RECOUP-1

Product stream side		
IN		
m_{in}	2119.0	mol/s
$mass_{in}$	138.4	kg/s
m_{H2SO4}	919.0	mol/s
m_{H2SO4}	0.4	mol %
Cp_{H2SO4}	125.0	J/mol K
m_{H2O}	769.0	mol/s
m_{H2O}	0.4	mol %
Cp_{H2O}	38.4	J/mol K
m_{SO3}	431.0	mol/s
m_{SO3}	0.2	mol %
Cp_{SO3}	72.3	J/mol K
Vap frac	1.0	frac
Liq frac	0.0	frac
Tin	775.0	K
UIT		
m_{uit}	2119.0	mol/s
$mass_{uit}$	138.4	kg/s
m_{H2SO4}	919.0	mol/s
m_{H2SO4}	0.4	mol %
m_{H2SO4}	90.1	kg/s
m_{H2O}	769.0	mol/s
m_{H2O}	0.4	mol %
m_{H2O}	13.8	kg/s
m_{SO3}	431.0	mol/s
m_{SO3}	0.2	mol %
m_{SO3}	34.5	kg/s
Vap frac	1.0	frac
Liq frac	0.0	frac
Tuit	775.0	K
T_{Cp}	0.8	
ΔT	0.0	K
Q	0.0	Watt
Q	0.0	MWt
Qvap	0.0	MWt
Qreaction	0.0	
Q_{TOT}	0.0	MWt

Heater stream side		
IN		
m_{in}	3357.0	mol/s
$mass_{in}$	138.3	kg/s
m_{SO3}	605.0	mol/s
m_{SO3}	0.3	mol %
Cp_{SO3}	73.8	J/mol K
m_{H2SO4}	34.0	mol/s
m_{H2SO4}	0.0	mol %
Cp_{H2SO4}	128.0	J/mol K
m_{SO2}	710.0	mol/s
m_{SO2}	0.1	mol %
Cp_{SO2}	53.1	J/mol K
m_{O2}	355.0	mol/s
m_{O2}	0.1	mol %
Cp_{O2}	33.8	J/mol K
m_{H2O}	1653.0	mol/s
m_{H2O}	0.5	mol %
Cp_{H2O}	39.4	J/mol K
Tin	850.0	K
UIT		
m_{uit}	3357.0	mol/s
$mass_{uit}$	138.3	kg/s
m_{SO3}	605.0	mol/s
m_{SO3}	0.3	mol %
Cp_{SO3}	73.8	J/mol K
m_{H2SO4}	34.0	mol/s
m_{H2SO4}	0.0	mol %
Cp_{H2SO4}	128.0	J/mol K
m_{SO2}	710.0	mol/s
m_{SO2}	0.1	mol %
Cp_{SO2}	53.1	J/mol K
m_{O2}	355.0	mol/s
m_{O2}	0.1	mol %
Cp_{O2}	33.8	J/mol K
m_{H2O}	1653.0	mol/s
m_{H2O}	0.5	mol %
Cp_{H2O}	39.4	J/mol K
Tuit	850.0	K
T_{Cp}	0.9	
ΔT	0.0	K
Q	0.0	Watt
Qreaction	0.0	MWt
Q	0	MWt

Table 71: Decomposition mass balance - Case 2

RX-101 (H2SO4 REACTOR)		
IN		
m_{in}	2119	mol/s
$mass_{in}$	138	kg/s
m_{H2SO4}	919	mol/s
m_{H2SO4}	0.434	mol
Cp_{H2SO4}	126.02	J/mol K
m_{H2O}	769	mol/s
m_{H2O}	0.363	mol
Cp_{H2O}	38.72	J/mol K
m_{SO3}	431	mol/s
m_{SO3}	0.203	mol %
Cp_{SO3}	38.72	J/mol K
Tin	775	K
UIT		
m_{uit}	2377.0	mol/s
$mass_{uit}$	138.4	kg/s
m_{SO3}	689.0	mol/s
m_{SO3}	0.3	mol %
m_{SO3}	55.2	kg/s
m_{H2O}	1027.0	mol/s
m_{H2O}	0.4	mol %
m_{H2O}	18.5	kg/s
m_{H2SO4}	661.0	mol/s
m_{H2SO4}	0.3	mol %
m_{H2SO4}	64.8	kg/s
Tuit	823.2	K
$\mathbf{T_{Cp}}$	0.8	
ΔT	-48.2	K
Q	7010117.0	Watt
Qheating	7.0	MWt
Qreaction	25.2	MWt
Qvap	0.0	MWt
Q_{TOT}	32.2	MWt
Conversion	1.0	

Table 72: Decomposition mass balance - Case 2

EX-102 (RECOUP-2)

Product stream side			
IN			
m_{in}	2377.0	mol/s	
$mass_{in}$	138.4	kg/s	
m_{H2SO4}	661.0	mol/s	
m_{H2SO4}	0.3	mol %	
Cp_{H2SO4}	131.4	J/mol K	
m_{H2O}	1027.0	mol/s	
m_{H2O}	0.4	mol %	
Cp_{H2O}	40.7	J/mol K	
m_{SO3}	689.0	mol/s	
m_{SO3}	0.3	mol %	
Cp_{SO3}	75.4	J/mol K	
Vap frac	1.0	frac	
Liq frac	0.0	frac	
Tin	823.2	K	
UIT			
m_{uit}	1688.0	mol/s	
$mass_{uit}$	138.5	kg/s	
m_{H2SO4}	52.0	mol/s	
m_{H2SO4}	0.0	mol %	
m_{H2SO4}	5.1	kg/s	
m_{H2O}	1636.0	mol/s	
m_{H2O}	0.5	mol %	
m_{H2O}	29.4	kg/s	
m_{SO3}	1298.0	mol/s	
m_{SO3}	0.4	mol %	
m_{SO3}	103.9	kg/s	
Vap frac	1.0	frac	
Liq frac	0.0	frac	
Tuit	1093.2	K	
T_{Cp}	1.0		
ΔT	-270.1	K	
Q	48794704.8	Watt	
Q	48.8	MWt	Stream heating
Qvap	0.0	MWt	
Qreaction	59.4	MWt	Reaction heat
Qheating	48.8	MWt	

Heater		
IN		
m_{in}	3357.0	mol/s
$mass_{in}$	138.3	kg/s
m_{SO3}	605.0	mol/s
m_{SO3}	0.2	mol %
Cp_{SO3}	75.9	J/mol K
m_{H2SO4}	34.0	mol/s
m_{H2SO4}	0.0	mol %
Cp_{H2SO4}	132.5	J/mol K
m_{SO2}	710.0	mol/s
m_{SO2}	0.2	mol %
Cp_{SO2}	54.4	J/mol K
m_{O2}	355.0	mol/s
m_{O2}	0.1	mol %
Cp_{O2}	34.5	J/mol K
m_{H2O}	1653.0	mol/s
m_{H2O}	0.5	mol %
Cp_{H2O}	41.2	J/mol K
Tin	1143.2	K
UIT		
m_{uit}	3357.0	mol/s
$mass_{uit}$	138.3	kg/s
m_{SO3}	605.0	mol/s
m_{SO3}	0.2	mol %
Cp_{SO3}	75.9	J/mol K
m_{H2SO4}	34.0	mol/s
m_{H2SO4}	0.0	mol %
Cp_{H2SO4}	132.5	J/mol K
m_{SO2}	710.0	mol/s
m_{SO2}	0.2	mol %
Cp_{SO2}	54.4	J/mol K
m_{O2}	355.0	mol/s
m_{O2}	0.1	mol %
Cp_{O2}	34.5	J/mol K
m_{H2O}	1653.0	mol/s
m_{H2O}	0.5	mol %
Cp_{H2O}	41.2	J/mol K
Tuit	850.0	K
T_{Cp}	1.0	
ΔT	293.2	K
Q	49677308.1	Watt
Q	49.7	MWt
Qreaction	0.0	
Q	49.7	MWt

Reaction		
IN		
m_{in}	3357.0	mol/s
$mass_{in}$	138.3	kg/s
m_{SO3}	605.0	mol/s
m_{SO3}	0.2	mol %
Cp_{SO3}	75.9	J/mol K
m_{H2SO4}	34.0	mol/s
m_{H2SO4}	0.0	mol %
Cp_{H2SO4}	132.5	J/mol K
m_{SO2}	710.0	mol/s
m_{SO2}	0.2	mol %
Cp_{SO2}	54.4	J/mol K
m_{O2}	355.0	mol/s
m_{O2}	0.1	mol %
Cp_{O2}	34.5	J/mol K
m_{H2O}	1653.0	mol/s
m_{H2O}	0.5	mol %
Cp_{H2O}	41.2	J/mol K
Tin	1143.2	K
UIT		
m_{uit}	3357.0	mol/s
$mass_{uit}$	138.3	kg/s
m_{SO3}	499.1	mol/s
m_{SO3}	0.2	mol %
Cp_{SO3}	75.9	J/mol K
m_{H2SO4}	139.9	mol/s
m_{H2SO4}	0.0	mol %
Cp_{H2SO4}	132.5	J/mol K
m_{SO2}	710.0	mol/s
m_{SO2}	0.2	mol %
Cp_{SO2}	54.4	J/mol K
m_{O2}	355.0	mol/s
m_{O2}	0.1	mol %
Cp_{O2}	34.5	J/mol K
m_{H2O}	1547.1	mol/s
m_{H2O}	0.5	mol %
Cp_{H2O}	41.2	J/mol K
Tuit	850.0	K
T_{Cp}	1.0	
ΔT	293.2	K
Q	49677308.1	Watt
Q	49.7	MWt
Qreaction	10.7	
Q	10.7	MWt

Table 73: Decomposition mass balance - Case 2

RX-102 (SO3 REACTOR)		
IN		
m_{in}	3003	mol/s
$mass_{in}$	138	kg/s
m_{SO3}	1316	mol/s
m_{SO3}	0.438	mol %
Cp_{SO3}	77.43	J/mol K
m_{H2O}	1653	mol/s
m_{H2O}	0.55	mol %
Cp_{H2O}	43.06	J/mol K
m_{H2SO4}	34	mol/s
m_{H2SO4}	0.01	mol %
Cp_{H2SO4}	136.26	J/mol K
Tin	1143.15	K
UIT		
m_{uit}	3357	mol/s
$mass_{uit}$	138	kg/s
m_{SO3}	605	mol/s
m_{SO3}	0.20	mol %
m_{SO3}	48.44	kg/s
m_{H2O}	1653	mol/s
m_{H2O}	0.48	mol %
m_{H2O}	29.75	kg/s
m_{O2}	355	mol/s
m_{O2}	0.09	mol %
m_{O2}	11.36	kg/s
m_{SO2}	710	mol/s
m_{SO2}	0.18	mol %
m_{SO2}	45.44	kg/s
m_{H2SO4}	34	mol/s
m_{H2SO4}	0.05	mol %
m_{H2SO4}	3.33	kg/s
Tuit	1143.15	K
T_{Cp}	1.14315	
ΔT	0	K
Q	0	Watt
Qheating	0.000	MWt
Q	70332120	Watt
	70.33	MWt
Qreaction	0.00	MWt
Q_{TOT}	70	MWt
Conversion	0.540	

Detail mass balance of the decomposition section: Case 3

Table 74: Decomposition mass balance - Case 3

HX-103		
IN		
m_{in}	1687.5	mol/s
$mass_{in}$	138.4	kg/s
m_{H2SO4}	1350.0	mol/s
m_{H2SO4}	0.8	mol
Cp_{H2SO4}	122.3	J/mol K
m_{H2O}	337.5	mol/s
m_{H2O}	0.2	mol
Cp_{H2O}	37.7	J/mol K
Tin	610.0	K
UIT		
m_{uit}	2204.0	mol/s
$mass_{uit}$	138.4	kg/s
m_{SO3}	517.0	mol/s
m_{SO3}	0.2	mol %
m_{SO3}	41.4	kg/s
m_{H2O}	854.0	mol/s
m_{H2O}	0.4	mol %
m_{H2O}	15.4	kg/s
m_{H2SO4}	833.0	mol/s
m_{H2SO4}	0.4	mol %
m_{H2SO4}	81.6	kg/s
Vapour	1.0	frac
Liquid	0.0	frac
Tuit	823.0	K
T_{Cp}	0.7	
ΔT	-213.0	K
Q	37880550.1	Watt
Q	37.9	MWt
Qvap	84.2	MWt
Qreaction	50.4	MWt
Q_{TOT}	172.5	MWt

Table 75: Decomposition mass balance - Case 3

EX-101 (RECOUP-1)

Product stream side		
IN		
m_{in}	2204.0	mol/s
$mass_{in}$	138.4	kg/s
m_{H2SO4}	833.0	mol/s
m_{H2SO4}	0.4	mol %
Cp_{H2SO4}	127.0	J/mol K
m_{H2O}	854.0	mol/s
m_{H2O}	0.4	mol %
Cp_{H2O}	39.0	J/mol K
m_{SO3}	517.0	mol/s
m_{SO3}	0.2	mol %
Cp_{SO3}	73.3	J/mol K
Vap frac	1.0	frac
Liq frac	0.0	frac
Tin	823.0	K
UIT		
m_{uit}	2204.0	mol/s
$mass_{uit}$	138.4	kg/s
m_{H2SO4}	833.0	mol/s
m_{H2SO4}	0.4	mol %
m_{H2SO4}	81.6	kg/s
m_{H2O}	854.0	mol/s
m_{H2O}	0.4	mol %
m_{H2O}	15.4	kg/s
m_{SO3}	517.0	mol/s
m_{SO3}	0.2	mol %
m_{SO3}	41.4	kg/s
Vap frac	1.0	frac
Liq frac	0.0	frac
Tuit	823.0	K
T_{Cp}	0.8	
ΔT	0.0	K
Q	0.0	Watt
Q	0.0	MWt
Qvap	0.0	MWt
Qreaction	0.0	
Q_{TOT}	0.0	MWt

Heater stream side		
IN		
m_{in}	3065.0	mol/s
$mass_{in}$	138.4	kg/s
m_{SO3}	504.0	mol/s
m_{SO3}	0.3	mol %
Cp_{SO3}	74.8	J/mol K
m_{H2SO4}	264.0	mol/s
m_{H2SO4}	0.0	mol %
Cp_{H2SO4}	130.0	J/mol K
m_{SO2}	582.0	mol/s
m_{SO2}	0.1	mol %
Cp_{SO2}	53.7	J/mol K
m_{O2}	291.0	mol/s
m_{O2}	0.1	mol %
Cp_{O2}	34.1	J/mol K
m_{H2O}	1424.0	mol/s
m_{H2O}	0.5	mol %
Cp_{H2O}	40.1	J/mol K
Tin	911.7	K
UIT		
m_{uit}	3065.0	mol/s
$mass_{uit}$	138.4	kg/s
m_{SO3}	504.0	mol/s
m_{SO3}	0.3	mol %
Cp_{SO3}	74.8	J/mol K
m_{H2SO4}	264.0	mol/s
m_{H2SO4}	0.0	mol %
Cp_{H2SO4}	130.0	J/mol K
m_{SO2}	582.0	mol/s
m_{SO2}	0.1	mol %
Cp_{SO2}	53.7	J/mol K
m_{O2}	291.0	mol/s
m_{O2}	0.1	mol %
Cp_{O2}	34.1	J/mol K
m_{H2O}	1424.0	mol/s
m_{H2O}	0.5	mol %
Cp_{H2O}	40.1	J/mol K
Tuit	911.7	K
T_{Cp}	0.9	
ΔT	0.0	K
Q	0.0	Watt
Qreaction	0.0	MWt
Q	0.0	MWt

Table 76: Decomposition mass balance - Case 3

RX-101 (H2SO4 REACTOR)		
IN		
m_{in}	2204.0	mol/s
$mass_{in}$	138.4	kg/s
m_{H2SO4}	833.0	mol/s
m_{H2SO4}	0.4	mol
Cp_{H2SO4}	127.0	J/mol K
m_{H2O}	854.0	mol/s
m_{H2O}	0.4	mol
Cp_{H2O}	39.0	J/mol K
m_{SO3}	517.0	mol/s
m_{SO3}	0.2	mol %
Cp_{SO3}	39.0	J/mol K
Tin	823.0	K
UIT		
m_{uit}	2205.0	mol/s
$mass_{uit}$	138.4	kg/s
m_{SO3}	518.0	mol/s
m_{SO3}	0.2	mol %
m_{SO3}	41.5	kg/s
m_{H2O}	855.0	mol/s
m_{H2O}	0.4	mol %
m_{H2O}	15.4	kg/s
m_{H2SO4}	832.0	mol/s
m_{H2SO4}	0.4	mol %
m_{H2SO4}	81.5	kg/s
Tuit	823.2	K
T_{Cp}	0.8	
ΔT	-0.1	K
Q	20863.2	Watt
Q	0.0	MWt
Qreaction	0.1	MWt
Qvap	0.0	MWt
Q_{TOT}	0.1	MWt
Conversion	0.9	

Table 77: Decomposition mass balance - Case 3

EX-102 (RECOUP-2)

Product stream side		
IN		
m_{in}	2205.0	mol/s
$mass_{in}$	138.4	kg/s
m_{H2SO4}	832.0	mol/s
m_{H2SO4}	0.4	mol %
Cp_{H2SO4}	130.5	J/mol K
m_{H2O}	855.0	mol/s
m_{H2O}	0.4	mol %
Cp_{H2O}	40.3	J/mol K
m_{SO3}	518.0	mol/s
m_{SO3}	0.2	mol %
Cp_{SO3}	75.0	J/mol K
Vap frac	1.0	frac
Liq frac	0.0	frac
Tin	823.2	K
UIT		
m_{uit}	1688.0	mol/s
$mass_{uit}$	138.5	kg/s
m_{H2SO4}	181.0	mol/s
m_{H2SO4}	0.1	mol %
m_{H2SO4}	17.7	kg/s
m_{H2O}	1507.0	mol/s
m_{H2O}	0.5	mol %
m_{H2O}	27.1	kg/s
m_{SO3}	1169.0	mol/s
m_{SO3}	0.4	mol %
m_{SO3}	93.6	kg/s
Vap frac	1.0	frac
Liq frac	0.0	frac
Tuit	1028.2	K
T_{Cp}	0.9	
ΔT	-205.1	K
Q	37292713.4	Watt
Qheating	37.3	MWt
Qvap	0.0	MWt
Qreaction	63.5	
Q_{TOT}	37.3	MWt

Heater		
IN		
m_{in}	3255.0	mol/s
$mass_{in}$	138.3	kg/s
m_{SO3}	695.0	mol/s
m_{SO3}	0.2	mol %
Cp_{SO3}	76.3	J/mol K
m_{H2SO4}	72.0	mol/s
m_{H2SO4}	0.0	mol %
Cp_{H2SO4}	133.3	J/mol K
m_{SO2}	582.0	mol/s
m_{SO2}	0.2	mol %
Cp_{SO2}	54.7	J/mol K
m_{O2}	291.0	mol/s
m_{O2}	0.1	mol %
Cp_{O2}	34.6	J/mol K
m_{H2O}	1615.0	mol/s
m_{H2O}	0.5	mol %
Cp_{H2O}	41.6	J/mol K
Tin	1143.2	K
UIT		
m_{uit}	3255.0	mol/s
$mass_{uit}$	138.3	kg/s
m_{SO3}	504.0	mol/s
m_{SO3}	0.2	mol %
Cp_{SO3}	76.3	J/mol K
m_{H2SO4}	264.0	mol/s
m_{H2SO4}	0.1	mol %
Cp_{H2SO4}	133.3	J/mol K
m_{SO2}	582.0	mol/s
m_{SO2}	0.2	mol %
Cp_{SO2}	54.7	J/mol K
m_{O2}	291.0	mol/s
m_{O2}	0.1	mol %
Cp_{O2}	34.6	J/mol K
m_{H2O}	1424.0	mol/s
m_{H2O}	0.5	mol %
Cp_{H2O}	41.6	J/mol K
Tuit	911.7	K
T_{Cp}	1.0	
ΔT	231.5	K
Q	39739268.4	Watt
Qcooling	39.7	MWt
Q	39.7	MWt

Reaction		
IN		
m_{in}	3255.0	mol/s
$mass_{in}$	138.3	kg/s
m_{SO3}	695.0	mol/s
m_{SO3}	0.2	mol %
Cp_{SO3}	76.3	J/mol K
m_{H2SO4}	72.0	mol/s
m_{H2SO4}	0.0	mol %
Cp_{H2SO4}	133.3	J/mol K
m_{SO2}	582.0	mol/s
m_{SO2}	0.2	mol %
Cp_{SO2}	54.7	J/mol K
m_{O2}	291.0	mol/s
m_{O2}	0.1	mol %
Cp_{O2}	34.6	J/mol K
m_{H2O}	1615.0	mol/s
m_{H2O}	0.5	mol %
Cp_{H2O}	41.6	J/mol K
Tin	1143.2	K
UIT		
m_{uit}	3255.0	mol/s
$mass_{uit}$	138.3	kg/s
m_{SO3}	504.0	mol/s
m_{SO3}	0.2	mol %
Cp_{SO3}	76.3	J/mol K
m_{H2SO4}	264.0	mol/s
m_{H2SO4}	0.1	mol %
Cp_{H2SO4}	133.3	J/mol K
m_{SO2}	582.0	mol/s
m_{SO2}	0.2	mol %
Cp_{SO2}	54.7	J/mol K
m_{O2}	291.0	mol/s
m_{O2}	0.1	mol %
Cp_{O2}	34.6	J/mol K
m_{H2O}	1424.0	mol/s
m_{H2O}	0.5	mol %
Cp_{H2O}	41.6	J/mol K
Tuit	911.7	K
T_{Cp}	1.0	
ΔT	231.5	K
Q	39739268.4	Watt
Qreaction	19.4	MWt
Q	19.4	MWt

Table 78: Decomposition mass balance - Case 3

RX-102 (SO3 REACTOR)		
IN		
m_{in}	2874.0	mol/s
$mass_{in}$	138.5	kg/s
m_{SO3}	1186.0	mol/s
m_{SO3}	0.4	mol %
Cp_{SO3}	76.9	J/mol K
m_{H2O}	1524.0	mol/s
m_{H2O}	0.5	mol %
Cp_{H2O}	42.4	J/mol K
m_{H2SO4}	164.0	mol/s
m_{H2SO4}	0.1	mol %
Cp_{H2SO4}	135.0	J/mol K
Tin	1040.0	K
UIT		
m_{uit}	3255.0	mol/s
$mass_{uit}$	138.3	kg/s
m_{SO3}	695.0	mol/s
m_{SO3}	0.2	mol %
m_{SO3}	55.6	kg/s
m_{H2O}	1615.0	mol/s
m_{H2O}	0.5	mol %
m_{H2O}	29.1	kg/s
m_{O2}	291.0	mol/s
m_{O2}	0.1	mol %
m_{O2}	9.3	kg/s
m_{SO2}	582.0	mol/s
m_{SO2}	0.2	mol %
m_{SO2}	37.2	kg/s
m_{H2SO4}	72.0	mol/s
m_{H2SO4}	0.0	mol %
m_{H2SO4}	7.1	kg/s
Tuit	1143.2	K
T_{Cp}	1.1	
ΔT	-103.2	K
Q	18362758.0	Watt
Q	18.4	MWt
Q	53518816.1	Watt
	53.5	MWt
Qreaction	9.0	MWt
Q_{TOT}	80.9	MWt
Conversion	0.5	

Detail mass balance of the decomposition section: Case 4

Table 79: Decomposition mass balance - Case 4

HX-103		
IN		
m_{in}	1687.5	mol/s
$mass_{in}$	138.4	kg/s
m_{H2SO4}	1350.0	mol/s
m_{H2SO4}	0.8	mol
Cp_{H2SO4}	117.5	J/mol K
m_{H2O}	337.5	mol/s
m_{H2O}	0.2	mol
Cp_{H2O}	36.7	J/mol K
Tin	610.0	K
UIT		
m_{uit}	2143.0	mol/s
$mass_{uit}$	138.4	kg/s
m_{SO3}	456.0	mol/s
m_{SO3}	0.2	mol %
m_{SO3}	36.5	kg/s
m_{H2O}	793.0	mol/s
m_{H2O}	0.4	mol %
m_{H2O}	14.3	kg/s
m_{H2SO4}	894.0	mol/s
m_{H2SO4}	0.4	mol %
m_{H2SO4}	87.6	kg/s
Vapour	1.0	frac
Liquid	0.0	frac
Tuit	651.3	K
$\mathbf{T_{Cp}}$	0.6	
ΔT	-41.3	K
Q	7065161.1	Watt
Q	7.1	MWt
Qvap	84.2	MWt
Qreaction	44.5	MWt
Q_{TOT}	135.7	MWt

Table 80: Decomposition mass balance - Case 4

EX-101 (RECOUP-1)					
Product stream side			**Heater stream side**		
IN			**IN**		
m_{in}	2143.0	mol/s	m_{in}	3400.0	mol/s
$mass_{in}$	138.4	kg/s	$mass_{in}$	138.3	kg/s
m_{H2SO4}	894.0	mol/s	m_{SO3}	585.0	mol/s
m_{H2SO4}	0.4	mol %	m_{SO3}	0.2	mol %
Cp_{H2SO4}	120.4	J/mol K	Cp_{SO3}	74.2	J/mol K
m_{H2O}	793.0	mol/s	m_{H2SO4}	12.0	mol/s
m_{H2O}	0.4	mol %	m_{H2SO4}	0.0	mol %
Cp_{H2O}	37.3	J/mol K	Cp_{H2SO4}	128.8	J/mol K
m_{SO3}	456.0	mol/s	m_{SO2}	752.0	mol/s
m_{SO3}	0.2	mol %	m_{SO2}	0.2	mol %
Cp_{SO3}	69.8	J/mol K	Cp_{SO2}	53.3	J/mol K
Vap frac	1.0	frac	m_{O2}	376.0	mol/s
Liq frac	0.0	frac	m_{O2}	0.1	mol %
Tin	651.3	K	Cp_{O2}	33.9	J/mol K
UIT			m_{H2O}	1675.0	mol/s
m_{uit}	2532.0	mol/s	m_{H2O}	0.5	mol %
$mass_{uit}$	138.4	kg/s	Cp_{H2O}	39.7	J/mol K
m_{H2SO4}	506.0	mol/s	**Tin**	902.4	K
m_{H2SO4}	0.2	mol %	**UIT**		
m_{H2SO4}	49.6	kg/s	m_{uit}	3400.0	mol/s
m_{H2O}	1182.0	mol/s	$mass_{uit}$	138.3	kg/s
m_{H2O}	0.5	mol %	m_{SO3}	570.0	mol/s
m_{H2O}	21.3	kg/s	m_{SO3}	0.2	mol %
m_{SO3}	844.0	mol/s	Cp_{SO3}	74.2	J/mol K
m_{SO3}	0.3	mol %	m_{H2SO4}	28.0	mol/s
m_{SO3}	67.6	kg/s	m_{H2SO4}	0.0	mol %
Vap frac	1.0	frac	Cp_{H2SO4}	128.8	J/mol K
Liq frac	0.0	frac	m_{SO2}	752.0	mol/s
Tuit	708.1	K	m_{SO2}	0.2	mol %
T_{Cp}	0.7		Cp_{SO2}	53.3	J/mol K
ΔT	-56.8	K	m_{O2}	376.0	mol/s
Q	9600333.4	Watt	m_{O2}	0.1	mol %
Q	9.0	MWt	Cp_{O2}	33.9	J/mol K
Qvap	0.0	MWt	m_{H2O}	1660.0	mol/s
Qreaction	37.8	MWt	m_{H2O}	0.5	mol %
Q_{TOT}	46.8	MWt	Cp_{H2O}	39.7	J/mol K
			Tuit	843.6	K
			T_{Cp}	0.9	
			ΔT	58.8	K
			Q	9654555.3	Watt
			Q	9.7	MWt
			Qreaction	1.6	MWt
			Q	11.3	MWt

Table 81: Decomposition mass balance - Case 4

RX-101 (H2SO4 REACTOR)		
IN		
m_{in}	2532.0	mol/s
$mass_{in}$	138.4	kg/s
m_{H2SO4}	506.0	mol/s
m_{H2SO4}	0.2	mol
Cp_{H2SO4}	124.6	J/mol K
m_{H2O}	1182.0	mol/s
m_{H2O}	0.5	mol
Cp_{H2O}	38.3	J/mol K
m_{SO3}	844.0	mol/s
m_{SO3}	0.3	mol %
Cp_{SO3}	38.3	J/mol K
Tin	708.1	K
UIT		
m_{uit}	2943.0	mol/s
$mass_{uit}$	138.4	kg/s
m_{SO3}	1256.0	mol/s
m_{SO3}	0.4	mol %
m_{SO3}	100.6	kg/s
m_{H2O}	1593.0	mol/s
m_{H2O}	0.5	mol %
m_{H2O}	28.7	kg/s
m_{H2SO4}	94.0	mol/s
m_{H2SO4}	0.0	mol %
m_{H2SO4}	9.2	kg/s
Tuit	823.2	K
T_{Cp}	0.8	
ΔT	-115.1	K
Q	12463401.5	Watt
Q	12.5	MWt
Qreaction	39.6	MWt
Qvap	0.0	MWt
Q_{TOT}	52.1	MWt
Conversion	0.99	

Table 82: Decomposition mass balance - Case 4

EX-102 (RECOUP-2)

Product stream side		
IN		
m_{in}	2943.0	mol/s
$mass_{in}$	138.4	kg/s
m_{H2SO4}	94.0	mol/s
m_{H2SO4}	0.0	mol %
Cp_{H2SO4}	129.1	J/mol K
m_{H2O}	1593.0	mol/s
m_{H2O}	0.5	mol %
Cp_{H2O}	39.8	J/mol K
m_{SO3}	1256.0	mol/s
m_{SO3}	0.4	mol %
Cp_{SO3}	74.3	J/mol K
Vap frac	1.0	frac
Liq frac	0.0	frac
Tin	823.2	K
UIT		
m_{uit}	1688.0	mol/s
$mass_{uit}$	138.5	kg/s
m_{H2SO4}	19.0	mol/s
m_{H2SO4}	0.0	mol %
m_{H2SO4}	1.9	kg/s
m_{H2O}	1669.0	mol/s
m_{H2O}	0.6	mol %
m_{H2O}	30.0	kg/s
m_{SO3}	1331.0	mol/s
m_{SO3}	0.4	mol %
m_{SO3}	106.6	kg/s
Vap frac	1.0	frac
Liq frac	0.0	frac
Tuit	943.1	K
T_{Cp}	0.9	
ΔT	-120.0	K
Q	20256108.9	Watt
Q	20.3	MWt
Qvap	0.0	MWt
Qreaction	7.3	MWt
Q_{TOT}	27.6	MWt

Heater stream side		
IN		
m_{in}	3406.0	mol/s
$mass_{in}$	138.4	kg/s
m_{SO3}	590.0	mol/s
m_{SO3}	0.2	mol %
Cp_{SO3}	75.5	J/mol K
m_{H2SO4}	8.0	mol/s
m_{H2SO4}	0.0	mol %
Cp_{H2SO4}	131.6	J/mol K
m_{SO2}	752.0	mol/s
m_{SO2}	0.2	mol %
Cp_{SO2}	54.2	J/mol K
m_{O2}	376.0	mol/s
m_{O2}	0.1	mol %
Cp_{O2}	34.3	J/mol K
m_{H2O}	1680.0	mol/s
m_{H2O}	0.5	mol %
Cp_{H2O}	40.8	J/mol K
Tin	1023.2	K
UIT		
m_{uit}	3406.0	mol/s
$mass_{uit}$	138.4	kg/s
m_{SO3}	585.0	mol/s
m_{SO3}	0.2	mol %
Cp_{SO3}	75.5	J/mol K
m_{H2SO4}	12.0	mol/s
m_{H2SO4}	0.0	mol %
Cp_{H2SO4}	131.6	J/mol K
m_{SO2}	752.0	mol/s
m_{SO2}	0.2	mol %
Cp_{SO2}	54.2	J/mol K
m_{O2}	376.0	mol/s
m_{O2}	0.1	mol %
Cp_{O2}	34.3	J/mol K
m_{H2O}	1675.0	mol/s
m_{H2O}	0.5	mol %
Cp_{H2O}	40.8	J/mol K
Tuit	902.4	K
T_{Cp}	1.0	
ΔT	120.8	K
Q	20265670.0	Watt
Q	20.3	MWt
Qreaction	0.4	MWt
Q	20.7	MWt

Table 83: Decomposition mass balance - Case 4

RX-102 (SO3 REACTOR)		
IN		
m_{in}	3030.0	mol/s
$mass_{in}$	138.5	kg/s
m_{SO3}	1342.0	mol/s
m_{SO3}	0.4	mol %
Cp_{SO3}	76.2	J/mol K
m_{H2O}	1680.0	mol/s
m_{H2O}	0.6	mol %
Cp_{H2O}	41.6	J/mol K
m_{H2SO4}	8.0	mol/s
m_{H2SO4}	0.0	mol %
Cp_{H2SO4}	133.2	J/mol K
Tin	1023.2	K
UIT		
m_{uit}	3406.0	mol/s
$mass_{uit}$	138.4	kg/s
m_{SO3}	590.0	mol/s
m_{SO3}	0.2	mol %
m_{SO3}	47.2	kg/s
m_{H2O}	1680.0	mol/s
m_{H2O}	0.5	mol %
m_{H2O}	30.2	kg/s
m_{O2}	376.0	mol/s
m_{O2}	0.1	mol %
m_{O2}	12.0	kg/s
m_{SO2}	752.0	mol/s
m_{SO2}	0.2	mol %
m_{SO2}	48.1	kg/s
m_{H2SO4}	8.0	mol/s
m_{H2SO4}	0.0	mol %
m_{H2SO4}	0.8	kg/s
Tuit	1023.2	K
T_{Cp}	1.0	
ΔT	0.0	K
Q	0.0	Watt
Q	0.0	MWt
Q	74387840.0	Watt
	74.4	MWt
Q_{TOT}	74.4	MWt
Conversion	0.56	

11. Appendix D: Electrolyzer Supporting Documentation

Reversible Cell Potentials for the SO_2-Depolarized Electrolyzer

Sulfate-sulfite couple using sulfate anion and protons:
$2\,H^+ + SO_4^{=} + H_2(g) \rightarrow SO_2(aq) + 2\,H_2O(l)$

Free energies of formation at 298.15K, 1bar

species	$\Delta G°_f$, kJ/gmol
$SO_2(aq)$	-300.676
$H_2O(l)$	-237.129
H^+	0
$SO_4^{=}$	-744.53
$H_2(g)$	0

$\Delta_{rxn}G°$, kJ/gmol -30.404

Universal Gas Constant, R 8.314472 J/gmol-K
Faraday Constant, F 96485.34 C/gmol
Electron equivalents in reaction, n 2
Molecular weight of water, M_{H_2O} 18.01534 g/gmol

Standard potential, $E°$ 0.15756 V

Nernst equation:
$E = E° - (RT/nF) \ln Q$
where
$Q = (\text{activity of } SO_2(aq))(\text{activity of } H_2O(l))^2 / [(10^{-pH})^2(\text{activity of } SO_4^{=})(\text{activity of } H_2(g))]$

Nernst potentials calculated from Aspen Plus simulation results using OLI-MSE properties

$(\partial E°/\partial T) = 0.784/1000$ V/K

Species concentrations, solution pH, and activity and fugacity coefficients calculated using OLI MSE properties model
Reversible cell potentials calculated using the Nernst equation
$E_T = E°_T - (RT/nF)\ln Q_T$, where $Q_T = [(a_{SO_2})(a_{H_2O})^2]/[(a_{SO_4})(a_{H_2})(10^{-pH})^2]$
$E°_T = E° + (T - 298.15)(\partial E°/\partial T)$

wt% sulfuric acid	Temperature, °C	System pressure, bar	SO_2 mass flow rate, kg/sec	Acid mass flow rate, kg/sec	SO_2 molality in anolyte, gmol/kg H_2O	SO_2 molal activity coefficient	activity of water	SO_4^{--} molality in anolyte, gmol/kg H_2O	SO_4^{--} molal activity coefficient	partial pressure of H_2, bar	H_2 fugacity coefficient	H_3O^+ molality in anolyte, gmol/kg H_2O	H_3O^+ molal activity coefficient	controlling equilibr.	SO_2 content g/100 g acid	molal activity of $SO_2(aq)$	activity of water	calculated pH	molal activity of H^+	molal activity of SO_4^{--}	activity of $H_2(g)$	Reversible cell potential, V
56	100	1	0.127288	33.1859	0.161761	0.687391	0.348005	1.417106	0.000529	0.090914	1.010332	18.539757	2.936492	VLE	0.384	0.124939	0.348005	-2.19668	157.2837	0.00075	0.091853541	0.292
56	100	1.5	0.227055	33.1859	0.32431	0.678983	0.347438	1.431967	0.000535	0.482479	1.00899	18.659666	2.896147	VLE	0.684	0.220201	0.347438	-2.19185	155.5418	0.000767	0.486816935	0.310
56	100	2	0.328434	33.1859	0.46924	0.670582	0.34687	1.447187	0.000541	0.980098	1.007257	18.690053	2.855775	VLE	0.980	0.314664	0.34687	-2.18694	153.7928	0.000784	0.987200307	0.316
56	100	3	0.536315	33.1859	0.766682	0.653766	0.345732	1.478733	0.000554	1.97741	1.005815	18.722291	2.774953	VLE	1.616	0.501231	0.345732	-2.17688	150.2711	0.00082	1.988909692	0.320
56	100	4	0.751497	33.1859	1.074934	0.63692	0.344589	1.511664	0.000568	2.975757	1.005387	18.786632	2.693986	VLE	2.265	0.684648	0.344589	-2.16648	146.7169	0.000858	2.991797159	0.321
56	100	5	0.974632	33.1859	1.384981	0.620033	0.343443	1.546729	0.000582	3.974521	1.005364	18.813283	2.612817	VLE	2.937	0.864934	0.343443	-2.15572	143.1262	0.000901	3.995842089	0.322
56	100	7	1.447679	33.1859	2.075158	0.586065	0.341135	1.622473	0.000614	5.972575	1.005841	18.914513	2.449575	VLE	4.363	1.216179	0.341135	-2.13296	135.8189	0.000997	6.007462567	0.323
56	100	9	1.96366	33.1859	2.818705	0.551705	0.338802	1.707794	0.000652	7.970951	1.006628	19.028437	2.284531	VLE	5.917	1.556094	0.338802	-2.10825	128.3083	0.001113	8.023783871	0.324
56	100	11	2.532593	33.1858	3.641716	0.516735	0.336437	1.805335	0.000696	9.96948	1.007557	19.158534	2.116732	VLE	7.632	1.881802	0.336437	-2.08112	120.5383	0.001257	10.04481809	0.325
56	100	13	3.170238	33.1859	4.56786	0.480842	0.33403	1.919017	0.00075	11.96813	1.008563	19.309963	1.944806	VLE	9.553	2.196417	0.33403	-2.05087	112.4276	0.001439	12.07060366	0.326
56	100	15	3.900838	33.1859	5.634146	0.443548	0.331568	2.055059	0.000817	13.9667	1.009615	19.480993	1.766675	VLE	11.755	2.499017	0.331568	-2.01642	103.8827	0.001679	14.10098593	0.326
56	100	17	4.706029	33.1659	6.904424	0.404046	0.32903	2.224342	0.000905	15.96529	1.010098	19.715923	1.578814	VLE	14.362	2.789708	0.32903	-1.97591	94.60458	0.002013	16.13609376	0.327
56	100	17.69399	15.71544	100	7.567482	0.385311	0.327863	2.315812	0.000955	16.85879	1.01119	19.837332	1.490116	VLLE	15.715	2.915832	0.327863	-1.95501	90.15947	0.002211	17.04743605	0.327
56	100	18	5.068107	32.24921	7.567519	0.385305	0.327861	2.315951	0.000955	16.98473	1.011248	19.837583	1.490064	LLE	15.71544	2.915802	0.327861	-1.955	90.15804	0.002212	17.15555157	0.327
56	100	20	5.068073	32.2488	7.56791	0.385206	0.327849	2.318629	0.000956	18.98344	1.012362	19.841079	1.489013	LLE	15.716	2.915206	0.327849	-1.95479	90.11336	0.002217	19.19765878	0.329
56	100	22	5.06804	32.24839	7.568303	0.385108	0.327838	2.321106	0.000958	20.96217	1.013468	19.844574	1.487962	LLE	15.716	2.914612	0.327838	-1.95457	90.06874	0.002223	21.24492002	0.331
53	100	1	0.115782	31.75344	0.156225	0.724128	0.408434	1.339712	0.000866	0.090914	1.010332	16.103507	2.543772	VLE	0.365	0.113127	0.408434	-2.00128	100.2943	0.000893	0.091853387	0.277
53	100	1.5	0.21583	31.75344	0.291287	0.715373	0.407773	1.353982	0.000874	0.482478	1.00899	16.121867	2.508578	VLE	0.680	0.208386	0.407773	-1.99642	99.18014	0.000912	0.486815905	0.294

53	100	2	0.317468	31.75344	0.428586	0.706817	0.40711	1.368802	0.000681	0.980088	1.007257	16.140676	2.473361	VLE	1.000	0.302647	0.40711	-1.9915	98.06113	0.000933	0.987200307	0.300
53	100	3	0.525799	31.75344	0.710222	0.689089	0.405783	1.398921	0.000697	1.97741	1.005815	16.179668	2.402859	VLE	1.656	0.489406	0.405783	-1.9814	95.80642	0.000975	1.988909682	0.303
53	100	4	0.741323	31.75344	1.001912	0.671532	0.404453	1.430788	0.000714	2.975757	1.006387	16.220634	2.332236	VLE	2.335	0.672616	0.404453	-1.97097	93.53461	0.001022	2.991787149	0.305
53	100	5	0.964677	31.75344	1.304565	0.65393	0.403118	1.464357	0.000732	3.974521	1.005364	16.26377	2.261437	VLE	3.038	0.953094	0.403118	-1.96017	91.23745	0.001072	3.995841727	0.306
53	100	7	1.437915	31.75344	1.947078	0.618526	0.400435	1.537338	0.000772	5.972575	1.005841	16.357489	2.119073	VLE	4.528	1.204319	0.400435	-1.93733	86.56254	0.001187	6.007461864	0.307
53	100	9	1.952905	31.75344	2.648314	0.582714	0.397729	1.61988	0.000818	7.97095	1.006628	16.463137	1.975173	VLE	6.150	1.543211	0.397729	-1.91253	81.75803	0.001325	8.023782774	0.308
53	100	11	2.519948	31.75344	3.423013	0.546271	0.394992	1.713953	0.000873	9.969478	1.007557	16.583981	1.828831	VLE	7.936	1.869891	0.394992	-1.8853	76.7887	0.001496	10.04481578	0.308
53	100	13	3.154093	31.75344	4.292789	0.508871	0.392216	1.823974	0.000939	11.98813	1.008563	16.724874	1.679185	VLE	9.933	2.184475	0.392216	-1.85494	71.60384	0.001713	12.07060285	0.309
53	100	15	3.878678	31.75344	5.291286	0.470025	0.389387	1.955774	0.001022	13.96669	1.009615	16.883486	1.524187	VLE	12.215	2.487036	0.389387	-1.82038	66.12661	0.001990	14.10097816	0.309
53	100	18	5.231583	31.75344	7.170164	0.407045	0.384998	2.219796	0.001199	16.96473	1.011248	17.230767	1.274745	VLE	16.476	2.918582	0.384998	-1.75627	57.05175	0.002662	17.15555127	0.310
53	100	18.40727	17.17127	100	7.478947	0.397804	0.384384	2.265173	0.001231	17.37173	1.011474	17.288673	1.238406	VLLE	17.171	2.975114	0.384384	-1.74586	55.70072	0.002789	17.5710477	0.310
53	100	19	5.286628	30.78881	7.478962	0.397772	0.38438	2.265976	0.001232	17.96406	1.011803	17.289738	1.238113	LLE	17.17127	2.974922	0.38438	-1.74579	55.69132	0.002791	18.17611139	0.311
53	100	20	5.286923	30.78862	7.479322	0.397714	0.384378	2.267208	0.001233	18.96344	1.012362	17.291514	1.237591	LLE	17.172	2.974629	0.384378	-1.74568	55.67418	0.002795	19.19785878	0.312
53	100	22	5.287114	30.78824	7.480044	0.397597	0.384367	2.270115	0.001235	20.96217	1.013488	17.295065	1.236547	LLE	17.173	2.974044	0.384367	-1.74538	55.63993	0.002802	21.24492002	0.313
50	100	1	0.104212	30.43952	0.133719	0.758716	0.468146	1.229029	0.000821	0.090914	1.010332	13.941768	2.235635	VLE	0.342	0.101455	0.468146	-1.82334	66.57902	0.001008	0.091653193	0.263
50	100	1.5	0.204446	30.43952	0.262397	0.749665	0.467395	1.242441	0.000829	0.482477	1.00899	13.958456	2.204696	VLE	0.672	0.19671	0.467395	-1.8185	65.84191	0.00103	0.486814689	0.279
50	100	2	0.306241	30.43952	0.393144	0.740812	0.466643	1.258191	0.000838	0.980088	1.007257	13.97556	2.173732	VLE	1.006	0.291167	0.466643	-1.81359	65.10149	0.001053	0.987200297	0.285
50	100	3	0.51479	30.43952	0.661212	0.722489	0.465137	1.284723	0.000857	1.97741	1.005815	14.011044	2.111738	VLE	1.691	0.477718	0.465137	-1.80353	63.61067	0.001101	1.988908672	0.288
50	100	4	0.73039	30.43952	0.938639	0.704337	0.463628	1.31474	0.000877	2.975757	1.005387	14.048363	2.049627	VLE	2.399	0.661119	0.463628	-1.79313	62.10555	0.001153	2.991787139	0.289
50	100	5	0.953658	30.43952	1.226259	0.686141	0.462117	1.34639	0.000896	3.97452	1.005364	14.087697	1.987353	VLE	3.133	0.841386	0.462117	-1.78236	60.58468	0.001209	3.995841206	0.290
50	100	7	1.426121	30.43952	1.836029	0.649547	0.459084	1.415297	0.000945	5.972574	1.005841	14.173287	1.862105	VLE	4.665	1.192568	0.459084	-1.75958	57.4887	0.001338	6.007461229	0.291
50	100	9	1.93929	30.43952	2.500182	0.612541	0.456033	1.493189	0.001	7.970949	1.006628	14.268966	1.735465	VLE	6.371	1.531452	0.456033	-1.73485	54.30599	0.001493	8.023781435	0.292
50	100	11	2.503029	30.43952	3.232067	0.574895	0.452957	1.582528	0.001064	9.969476	1.007557	14.380767	1.606798	VLE	8.223	1.8581	0.452957	-1.70759	51.01364	0.001684	10.04481321	0.293
50	100	13	3.13168	30.43952	4.051308	0.536282	0.44985	1.686956	0.001142	11.96812	1.008563	14.51018	1.475058	VLE	10.288	2.172644	0.44985	-1.67741	47.5789	0.001926	12.07059335	0.293
50	100	15	3.847342	30.43952	4.968151	0.496208	0.4467	1.812203	0.001238	13.96669	1.009615	14.665262	1.338781	VLE	12.639	2.475161	0.4467	-1.64298	43.95245	0.002240	14.10097997	0.294
50	100	18	5.174225	30.43952	6.738138	0.431388	0.441864	2.063044	0.001442	16.96473	1.011248	14.975495	1.11994	VLE	16.998	2.80662	0.441864	-1.57929	37.95663	0.002976	17.15555137	0.295
50	100	18.97506	18.75692	100	7.449329	0.40824	0.440252	2.171289	0.001536	17.93916	1.011789	15.109242	1.042631	VLLE	18.757	3.041115	0.440252	-1.55367	35.7826	0.003334	18.15064846	0.295
50	100	19	5.483881	29.23661	7.449353	0.408238	0.44025	2.17133	0.001536	17.96406	1.011803	15.109346	1.042621	LLE	18.75692	3.041108	0.44025	-1.55367	35.78266	0.003334	18.17611139	0.295
50	100	20	5.484107	29.23636	7.449896	0.40817	0.440248	2.172803	0.001537	18.96344	1.012362	15.111168	1.042069	LLE	18.758	3.040624	0.440248	-1.55351	35.76921	0.003339	19.19785878	0.296
50	100	22	5.484541	29.23592	7.450983	0.408034	0.440244	2.175748	0.001539	20.96217	1.013488	15.114805	1.041065	LLE	18.760	3.040255	0.440244	-1.55318	35.74234	0.003349	21.24492002	0.297
0.1	100	20	35.25591	100	5.395	0.570075	0.92762	0.000593	0.19850	18.963	1.012362	0.154321	0.51160	VLE	35.256	3.075398	0.927625	1.070019	0.08511	0.000118	19.19785878	0.024
0.5	100	20	34.88198	100	5.376	0.572052	0.92686	0.002807	0.18104	18.963	1.012362	0.178664	0.50849	VLE	34.882	3.075561	0.926861	1.00627	0.098367	0.000508	19.19785878	0.052
1	100	20	34.45434	100	5.357	0.574121	0.92577	0.005284	0.16166	18.963	1.012362	0.216289	0.50571	VLE	34.454	3.075794	0.925767	0.929578	0.117604	0.000854	19.19785878	0.066
1.5	100	20	34.0771	100	5.342	0.575800	0.92453	0.007530	0.14461	18.963	1.012362	0.254832	0.50410	VLE	34.077	3.076058	0.924529	0.857146	0.138948	0.00109	19.19785878	0.075
2	100	20	33.72992	100	5.330	0.577160	0.92316	0.009627	0.13023	18.963	1.012362	0.297738	0.50356	VLE	33.730	3.076349	0.923161	0.789375	0.162414	0.001254	19.19785878	0.082
2.5	100	20	33.41682	100	5.321	0.578264	0.92168	0.011638	0.11762	18.963	1.012362	0.343488	0.50403	VLE	33.417	3.076664	0.921679	0.726212	0.18784	0.001369	19.19785878	0.089
3	100	20	33.12002	100	5.313	0.579186	0.92009	0.013808	0.10870	18.963	1.012362	0.391648	0.50524	VLE	33.120	3.077002	0.920095	0.66735	0.215105	0.001452	19.19785878	0.094
4	100	20	32.58042	100	5.302	0.580527	0.91665	0.017546	0.08886	18.963	1.012362	0.493920	0.51014	VLE	32.580	3.077734	0.916652	0.560881	0.274877	0.001559	19.19785878	0.103
5	100	20	32.0852	100	5.294	0.581474	0.91288	0.021826	0.07504	18.963	1.012362	0.602708	0.51724	VLE	32.085	3.078536	0.912887	0.466619	0.341492	0.001623	19.19785878	0.111
7.5	100	20	30.95668	100	5.286	0.582776	0.90223	0.033098	0.05144	18.963	1.012362	0.897594	0.54196	VLE	30.957	3.080805	0.902227	0.268271	0.539174	0.001703	19.19785878	0.127
10	100	20	29.91428	100	5.288	0.583144	0.88993	0.047327	0.03678	18.963	1.012362	1.221646	0.57314	VLE	29.914	3.083424	0.889926	0.10415	0.786774	0.001741	19.19785878	0.140
15	100	20	27.9754	100	5.311	0.581757	0.86058	0.089958	0.02011	18.963	1.012362	1.960074	0.64557	VLE	27.975	3.089629	0.860577	-0.16742	1.47036	0.001789	19.19785878	0.161
20	100	20	26.18938	100	5.387	0.577086	0.82487	0.160055	0.01157	18.963	1.012362	2.843843	0.72080	VLE	26.189	3.097273	0.824869	-0.39533	2.485046	0.001852	19.19785878	0.180
25	100	20	24.58993	100	5.477	0.567138	0.78259	0.284879	0.00693	18.963	1.012362	3.925478	0.78384	VLE	24.590	3.10627	0.782595	-0.59458	3.931731	0.001975	19.19785878	0.197
30	100	20	23.27553	100	5.683	0.548401	0.73340	0.505576	0.00441	18.963	1.012362	5.291164	0.81534	VLE	23.276	3.116739	0.733405	-0.76955	5.882297	0.002229	19.19785878	0.214
35	100	20	22.38169	100	6.057	0.516546	0.67627	0.874926	0.00310	18.963	1.012362	7.060129	0.80529	VLE	22.382	3.128897	0.676269	-0.92464	8.407057	0.002714	19.19785878	0.232
40	100	20	21.91829	100	6.658	0.472081	0.60863	1.384665	0.00247	18.963	1.012362	9.315548	0.78724	VLE	21.918	3.143288	0.608629	-1.08097	12.0494	0.003415	19.19785878	0.250
45	100	20	23.82862	100	7.452	0.424588	0.52971	1.900587	0.00208	18.963	1.012362	12.003634	0.82206	VLE	23.829	3.163885	0.529707	-1.27018	18.62858	0.003948	19.19785878	0.271