Technical evaluation of the copper chloride water splitting cycle

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Mini-dissertation submitted in partial fulfillment of the requirements for the degree
Master of Engineering at the Potchefstroom Campus of the North-West University

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November 2011

Acknowledgements

I wish to thank the following people who assisted me in writing this mini-dissertation.

My supervisor, Prof P.W.E. Blom, who gave me guidance while writing this, especially with my weird questions.

My fiancée, Yvette Bräsler, who sat and helped me edit and complete this document on many weekends.

My parents, Adv Pieter Kemp SC and Hilda Kemp, who encouraged me to continue with my masters and in the writing of this mini-dissertation.

Honeywell Ltd and Nick Meijer who sponsored Unisim^{TM} and assisted me in the development of the flow sheets used in this thesis.

Joe-Nimique Cilliers who allowed the many questions I had on her work and the electrolyser.

Prof Cecelia Jansen and Mr. Oswald Davies, for proofreading this mini-dissertation, your advice assisted me in making sure what I intend on writing actually does come out correctly.

Joyce Vilakazi, who brought me coffee while I was struggling to stay focused.

God, who gave me the intelligence and the discipline to follow through with this mini-dissertation

This mini-dissertation is dedicated to my father,

Adv Pieter Kemp SC,

who tragically died while I was writing this mini-dissertation,

Rest in peace dad.

Abstract

The global energy sector is facing a crisis caused by the increasing demand for energy. Non-renewable energy sources, such as fossil fuels produce greenhouse gases that are largely blamed for climate change. The Kyoto protocol requires industrialised nations to reduce their collective greenhouse gas emissions. Hydrogen as an alternative fuel can serve as a substitute.

Hydrogen production is expensive and the gas is largely derived from fossil fuels by a process that releases large quantities of greenhouse gases. In South Africa work on hydrogen production was first done on the Hybrid Sulphur cycle. The high operating temperature and highly corrosive environment involved in the process makes this cycle difficult to work with. The copper-chloride cycle has a lower operating temperature and uses less corrosive materials, making the cycle potentially more economical.

Evaluation of the cycle started with the development of four models: the Base model, the Canadian model (developed in Canada) the Kemp model and the Excess model. The Kemp model has the best overall efficiency of 40.89 %, producing hydrogen at a cost of US$4.48/kg. The model does not however provide the excess steam required for the cycle. The Excess model which is based on the Kemp model does provide the excess steam and produces an overall efficiency of 39 % and hydrogen at a cost of US$4.60/kg.

The copper-chloride cycle has an improved efficiency and produces hydrogen at a lower cost when compared to the hybrid sulphur cycle. The final conclusion of this thesis is that the copper-chloride cycle should be investigated further and an expected capital and operational costs estimate should be developed to obtain more accurate figures.

Keywords: copper-chloride cycle, hydrogen, nuclear, evaluation.

Opsomming

Die wêreldwye energie sektor het te kompe met ‘n krises wat veroorsaak word deur die toenemende vraag na energie. Nie-herniebare energiebronne, soos fossielbrandstof produseer kweekhuisgasse waaraan limaat veranderinge hoofsaaklik toegeskryf word. Die Kyotoprotokol vereis dat industriële lande hul kweekgasse moet verminder. Waterstof as ‘n alternatiewe brandstof kan dien as plaasvervanger.

Waterstofproduksie is duur en word hoofsaaklik verkry van fossielbrandstowwe deur middle van n proses wat groot hoeveelhede kweekgasse afgee. Waterstof produksie in Suid Afrika is vroeër deur middle van die hibriedswaelsiklus gelewer. Die hoë werkstemperatuur en korrosiewe omgewing maak dit ‘n baie moeilike siklus om mee te werk. Die koperchloorsiklus het n laer werkstemperatuur en gebruik minder korrosiewe chemikalieë wat die siklus economies meer voordelig maak.

Die evaluasie van die siklus begin met die ontwikkeling van vier modelle genaamd die Basismodel, die Kanadese model, die Kempmodel en die “Excess” model. Die Kempmodel het die beste algehele doeltreffenheid van 40.89% en lewer waterstof teen n koste van US$4.49/kg. Die model het egter nie die bykomende stoom wat benodig word vir die siklus beskikbaar nie. Die ”Excess” model, wat gebaseer is op die Kempmodel, lewer ekstra stoom, het ‘n algehele doeltreffenheid van 39 % en lewer waterstof teen US$4.60/kg.

Die koperchloorsiklus het n verbeterde doeltreffenheid en produseer waterstof teen n laer koste wanneer dit vergelyk word met die hibriedswaelsiklus. Die finale gevolgtrekking van hierdie mini-verhandeling is dat die koperchloorsiklus verder ondersoek moet word en ‘n verwagte kapitaal- en bedryfskoste moet beraam word om meer akkurate syfers te kry.

Sleutelwoorde: koper-kloor siklus, waterstof, kern, evaluasie.

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Abbreviations

A/cm2	Ampere per centimeter squared
AECL	Atomic Energy of Canada LTD
Bar	Pressure in bar
C	Coulomb
Cp	Heat capacity
g	gram
h	hour
kgmole	kilo mole
HHV	Higher Heating Value
HTGR	High-temperature gas reactor
HTSE	High-temperature steam electrolysis
HTR	High-temperature reactor
HyS	Hybrid sulphur cycle
˚K	degree Kelvin
kg	kilogram
I	Current measured in ampere
kJ	kilojoule
kPa	Pressure in kilopascals
LHV	Lower heating value
m^3	Volume in cubic metres

Mol	mole
MW	Megawatt
MWe	Megawatt electric
MWt	Megawatt thermal
P	Electrical power
PWh	Petawatt hour
SCWR	Supercritical water reactor
V	Volt
W	Watt
s	second
ΔH	Heat of reaction
%	percent
US$	US dollar
°C	degree Celsius
e^-	electron
°K	degree Kelvin
CO	carbon monoxide
CH_4	methane
CO_2	carbon dioxide
Cu	copper
CuCl	copper chloride

$CuCl_2$	copper dichloride
CuO	copper oxide
$CuO.CuCl_2$	copper oxychloride
$CuOHCl$	copper oxide hydrogen chloride
H_2	hydrogen
H_2O	water
HCl	hydrochloric acid
HI	hydrogen iodide
H_2SO_4	sulphuric acid
I_2	iodine
O_2	oxygen
SO2	sulphur dioxide
SO_3	sulphur Tri-oxide

1 Introduction

The global energy sector is facing a rapidly growing shortage of energy caused in particular by the depletion of non-renewable energy sources, global warming and climate change (Cilliers, 2010). Global warming and climate change are blamed on the use of fossil fuels which generate large volumes of greenhouse gases. To reduce the output of greenhouse gases a reduction in the use of oil, coal and other greenhouse gas emitting substances needs to be accomplished.

The Kyoto protocol was an accord to which industrialised countries subscribed in taken of a legally binding document to reduce their collective greenhouse gas emissions by 5.2 % compared to the year 1990 (Kyotoprotocol, 2011). This document gives rise to the search for alternative fuels which satisfy the following criteria (Cilliers, 2010):

- Technical feasibility
- Energy efficient production
- Sustainability
- Economically viable and competitive
- Clean and environmentally friendly

Hydrogen is a viable energy source.

In South Africa work in this regard was done on the Hybrid Sulphur (HyS) water splitting cycle. Disadvantages of the HyS cycle include the high operating temperature of 850 ˚C and a potentially highly corrosive environment. The purpose of this mini-dissertation is to do an evaluation of the copper-chloride (CuCl) water splitting cycle by determining whether it is viable to develop the cycle further and what the cost of production would be. The CuCl cycle has the advantages of requiring a maximum operating temperature of 530 ˚C and operates with less corrosive materials which results in a less corrosive environment.

1.1 Global energy outlook

The world's population is increasing; developing countries need a secure and steady supply of heat and electricity to develop more fully. Worldwide 135 PWh of energy was consumed in 2005 and the demand is estimated to grow to 203 PWh by 2030 (Cilliers, 2010) as shown in figure 1-1.

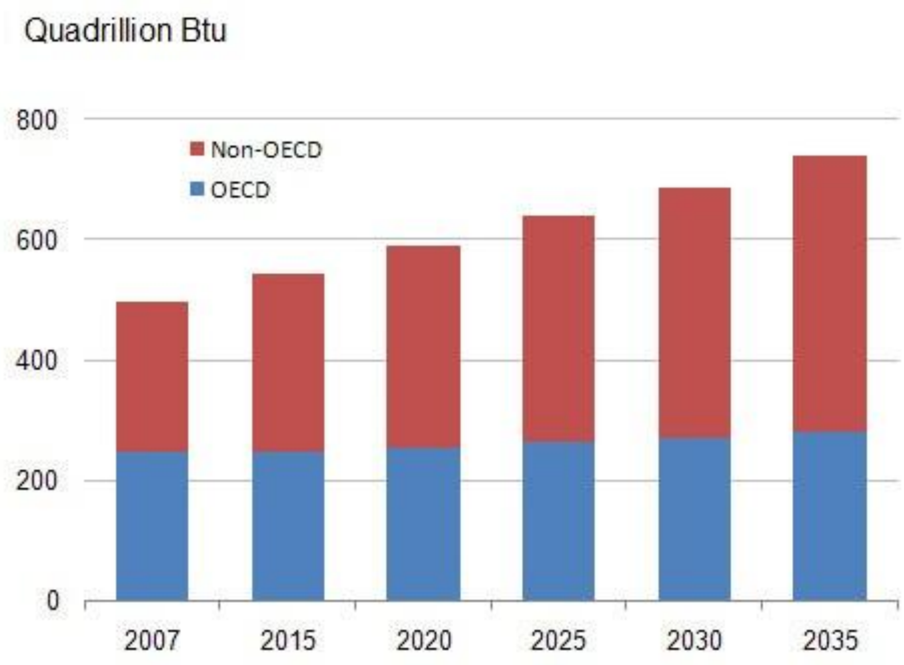

Figure 1-1: World energy consumption 2005 – 2030 (Cilliers, 2010)

For the foreseeable future, according to the International Energy Association (www.iea.org), the main source of energy in developing countries will be coal which produces greenhouse like carbon dioxide (CO_2). The International Energy Outlook estimates that energy demand worldwide will increase by 45 % between 2008 and 2030 with coal being responsible for more than a third of the overall increase (Cilliers, 2010), thus increasing the emissions of greenhouse gas accordingly. The Kyoto protocol was signed in December 1997 (Kyotoprotocol, 2011) to curb the increased use of coal and thereby fight global warming.

Despite this, according to the IEO 2010 reference case, carbon dioxide emissions will grow from 29.7 billion tons in 2007 to 33.8 billion tons in 2020 (IEA, 2010) with emissions in 2010 having reached 30.6 billion tonnes of CO_2 (Dawn, 2010). The increase in greenhouse gas emissions hastens development of the problem of rapid climate change and global warming.

The rapid increase in the world’s population together with technological advancements and diminishing fossil fuel reserves have increased the urgency of investigating and utilising alternative energy sources that promise to be more efficient and environmentally benign (Orhan, Dincer & Rosen, 2009). To successfully continue with this venture appropriate alternative energy sources, efficient technology for the production of energy from these sources and methods of storing and transporting the energy must be investigated (Cilliers, 2010).

Hydrogen has the potential to meet the challenges of serving as an alternative source of fuel. It is defined as an energy carrier which needs a primary source of energy, such as a nuclear reactor, for production (Orhan, Dincer & Rosen, 2008). Hydrogen can replace petroleum products for the automotive industry and limit the dependence on imported products, reducing the amount of carbon dioxide released and preparing for the eventuality that the oil may run out (Yildez & Kazimi, 2005).

Hydrogen production, based on fossil fuels, presents a number of key challenges. Currently hydrogen production is expensive, hence lower production costs and a sustainable energy source for large-scale hydrogen production is needed to stimulate a hydrogen economy (Wang, Naterer & Gabriel, 2008).

Nuclear power is an ideal energy source for use in the production of hydrogen. The challenges of hydrogen production can be met by using inherently safe, high-temperature reactors which have near-zero greenhouse gas emissions and, in combination with a thermochemical cycle, produce hydrogen in large quantities and at a competitive cost.

Nuclear power has a stable future fuel supply which can supply heat at the required temperatures for both the hybrid sulphur (HyS) and the CuCl cycles, neither of which produces greenhouse gases. Numerous studies have been done to determine the viability of other cycles, including the HyS water-splitting cycle coupled to a nuclear high-temperature reactor. This cycle has a potential thermal efficiency of 21 % to 31 % lower heating value and 25 % to 37 % higher heating value. Hydrogen is produced at an estimated cost between US$5.44/kg and US$7.67/kg. A disadvantage of the HyS cycle is the high operating temperature of 850 °C (Cilliers, 2010).

Hydrogen already has a significant market role in the production of fertilizers and in the oil market (Yildez & Kazimi, 2005). The worldwide demand for hydrogen for oil refineries and chemical plants has increased (Chukwe, Naterer & Rosen, 2008). A recent study on Sasol's Fischer-Tropsch process has shown potential to reduce carbon dioxide emissions by 75 % (Chiuta, 2008).

Many studies have been conducted in anticipation of the worldwide increase in total hydrogen demand over the next few years. It is expected that hydrogen will ultimately be used as an energy carrier in the transportation sector (Yildez & Kazimi, 2005). Hydrogen as an automotive fuel is encouraged by two strong global concerns, the substitution of increasingly scarce and costly fossil fuels and the abatement of air pollution (Orhan, Dincer & Rosen, 2008). Automakers such as BMW are investing significantly in hydrogen vehicles (BMW, 2011) with Japan having set a goal of having 5 million fuel-cell vehicles on the road by 2020
(Wang, Naterer & Gabriel, 2008).

1.2 Hydrogen economy

The birth of the hydrogen economy has been launched by the global energy crisis. The production of ammonia and the conversion of heavier crude oils to liquid fuels consumes upwards of 50 million tons of hydrogen each year (Forsberg, 2003). The worldwide hydrogen market in 2008 was estimated at US$282 billion/year (Wang, Gabriel & Naterer, 2008).

In recent years the concept of replacing fossil fuels with hydrogen has been discussed more often. A variety of methods for the production of hydrogen exist, notably steam-methane reforming, coal-gasification, electrolysis, high-temperature steam-electrolysis and thermochemical cycles (Cilliers, 2010).

Currently hydrogen is mainly produced by steam methane reforming which produces large quantities of greenhouse gases. Most of the processes mentioned above also emit large quantities of carbon dioxide either directly (steam methane) or indirectly (electrolysis using coal to generate electricity) during the production of hydrogen (Wang *et al.,* 2009). In the future, hydrogen will be produced using existing energy carriers with different primary energy carriers and sources (Orhan, Dincer & Rosen, 2008). Fossil fuels are expected to be replaced by hydrogen as a renewable energy source that will become a future energy carrier (Cilliers, 2010).

The emergence of the hydrogen economy will increase the demand for hydrogen as an energy carrier. Hydrogen will be a significant driving force as a sustainable future energy supply and a significant hydrogen economy is expected to rise in the transportation sector (BMW, 2011). Even with this expected emergence hydrogen would also be used for power generation, transportation and in the oil sands of Alberta (Rosen, 2009).

The rise in demand will require the world's hydrogen production capacity to increase. Servicing this demand must be done in a clean and sustainable manner (Naterer *et al.*, 2010).

Producing hydrogen in a clean, environmentally friendly manner, without using fossil fuels strengthens the case for using nuclear power as an energy source during production. Advanced nuclear reactor design, such as the third generation, inherently safe, helium-cooled graphite-moderated reactor (HTGR) which produces heat at 750 °C with no greenhouse gas emissions is ideal for use as an energy source. A combination of the copper-chloride cycle, which has no effluents, and the nuclear plant, which has no greenhouse gas emissions, this cycle can be considered environmentally friendly (Cilliers, 2010).

1.3 Hydrogen Background

Interest in hydrogen is growing as it is considered to be a useful and necessary chemical energy carrier (Orhan *et al.,* 2009). Hydrogen is the most abundant element in the universe and is the primary substance from which all matter and elements in the universe are made of. However, it mainly exists in combination with other elements. It is found naturally on earth mainly in the form of water (H_2O), natural gas (CH_4) and coal and oil.

Hydrogen is useful in that it is chemically active with an energy content of 120.7 GJ/ton, which is higher than that of any fossil fuel (Orhan, Dincer & Rosen, 2008). In modern industrial settings hydrogen is used in the production of ammonia, the refining of petroleum, methanol production and various other uses (Cilliers, 2010).

Hydrogen properties are more extreme than those of most gases:

- It is the lightest element with only one proton and one electron (Rosen, 2009).
- Highest thermal velocity and conductivity (Rosen, 2009).
- Lowest viscosity and density (Rosen, 2009).
- Among the highest energy yields at 122 kJ/g (Rosen, 2009).
- High specific energy content of 143 kJ/kg (Rosen, 2009).
- Boiling point is 20.3 °K (Rosen, 2009).
- It occurs naturally in both fossil fuels and water (Cilliers, 2010).
- Lowest molecular weight of any gas (Cilliers, 2010),

Hydrogen releases its potential chemical energy by combusting with air; the by-product of which is high potential heat and water. Hydrogen energy is also extracted by an electrochemical reactor where chemical energy is converted to electrical energy. As a fuel, hydrogen is cleaner than fossil fuels as it produces water and few, if any, other contaminants when burned in air or electrochemically combined with oxygen (Orhan, Dincer & Rosen, 2008).

The complete hydrogen fuel cycle is considered almost pollution free. Hydrogen has a relatively high ignition temperature, very low ignition energy and a wide flammability range. The combination of high combustion heat and low molecular weight has made hydrogen a prime fuel for the use in rocket propulsion (Rosen, 2009).

Hydrogen combustion engines and fuel cell technology has been advanced by the transportation sector and studies have been done (White, Steeper & Lutz, 2006). Hydrogen is highly efficient as a transportation fuel which produces non-toxic gas emissions in the form of water vapour (Cilliers, 2010) and has an advantage over other fuels in its high energy density and environmentally benign nature (Chukwe, Naterer & Rosen, 2008). Further, it can be stored in containers, pumped through pipelines and metered with control valves. Hydrogen is not as highly an active chemical as other chemicals used in batteries and has a unique advantage over electricity as it can be stored instead of having to be used as it is created (Rosen, 2009).

1.4 Problem statement

A quest for cleaner energies has been pursued for decades. Prices of oil, gas and coal are set to increase as are the high greenhouse gas emission levels of these fuels. A new, more environmentally friendly energy source needs to be found.

South Africa and North-West University have jointly set their sights on the hybrid sulphur cycle. As noted earlier, the cycle's biggest disadvantage is its high operating temperature of 850 ˚C which leads to high material strains, highly corrosive chemicals and expensive construction materials, advanced materials of construction, additional safety measures and higher construction cost will have to be provided if the high-temperature reactor has to achieve such a high temperature. Operating a lower temperature cycle (which splits water into its elements) is advantageous and needs to be investigated.

The copper-chloride cycle has two unique advantages. It operates at a relatively low temperature of 530 ˚C and with less corrosive materials and chemicals when compared to the HyS process. This combination will decrease the cost of specialised materials and therefore the cost concurred during construction of the high temperature reactor.

South Africa has only recently begun to study this new cycle. The purpose of the mini-dissertation presented here is to create a starting point for future studies of the CuCl cycle in South Africa, and to determine whether or not it is both thermally and economically viable for the purposes of future applications.

1.5 Research methodology

The evaluation consists in building a basic model with no heat transfer between processes. This is done in Unisim^{TM} with a hydrogen output basis of 1 kgmole/h for the following reasons:

- The fact that heat exchange values are either two- or three-digit heat-flow values makes it easier to compare the values of streams.
- Any changes in efficiency can be easily confirmed immediately.
- The amount of energy which is required for the electrolysis is dependent on the amount of hydrogen being formed. The energy requirement needs to be recalculated every time the hydrogen flow is changed. Thus if the number remains constant, the energy input will remain constant.

Once the basic model is built, models found in literature will be built in Unisim^{TM} and the thermal efficiencies will be calculated. If improvements can be made the model will be altered to determine whether or not there is an improvement on the new model. When all models have been tried, they will be scaled up to operate with a heat source of 350 MW of thermal energy.

Finally, a basic economic evaluation will be performed. As none of the few economic studies done on the CuCl cycle had the benefit detailed knowledge of the economic processes, the master thesis by Cilliers (2010) will be used to form a basis for the fixed capital costs to determine the economic viability of these models.

1.6 Focus of this study

The aim of this mini-dissertation is to investigate the suitability of the copper-chloride cycle for hydrogen production with particular reference to:

- Develop the Canadian built flowsheet preferably using the Unisim^{TM} engineering simulation package.
- Evaluate the flowsheet to determine its viability and operational parameters.
- Develop a unique model of the CuCl cycle to evaluate its viability and operational parameters.
- Calculate the hydrogen and oxygen production rates of the two flow sheets.
- Calculate the thermal efficiency of the cycle using the lower heating value of 122 MJ/kg.
- Determine the economic production cost of the cycle based on the fixed capital cost of Cilliers (2010).
- Compare the copper-chloride cycle’s thermal efficiency to the thermal efficiency and economics of the hybrid sulphur cycle.
- Simulate alternative models to further improve the cycle.

1.7 Outline of mini-dissertation

- Chapter 1: Gives a basic introduction on the current global energy outlook. Background on hydrogen and the hydrogen economy is introduced in this section. Finally the problem statement is given in this section.
- Chapter 2: Presents the literature survey. First covering different methods of producing hydrogen. The main topic of this mini-dissertation is presented and the cycle is described. The final section takes a more detailed look into each of the steps and presents a summary of information.
- Chapter 3: Presents the models which will be used to form the evaluation. Each of the cycles is presented individually. All the models are based on the first one. The following models have changes that will be explained.
- Chapter 4: The results and discussion are presented in the next chapter. The four main models are presented with their individual mass and energy balances. Three additional models were developed to test different add-ons to the cycle. Their mass and energy balances are shown here. The economic analysis is presented last to give an overall picture of the cost of each cycle. A discussion on the performance of the models and the overall performance is presented last.
- Chapter 5: The conclusion and recommendation will be presented following the results.

2. Literature survey

2.1 Hydrogen production methods

Hydrogen is generated from a variety of processes using a wide range of energy sources. These processes include the reforming of natural gas, gasification of coal, electrolysis of water and, more recently, thermochemical water-splitting cycles (Rosen, 2009). The main sources of hydrogen have been natural gas, petroleum and water (Yalcin, 1989).

Hydrogen is an energy carrier that needs to be produced from a primary energy source. A proposed method is to use nuclear heat with the aid of some intermediary steps as energy source, to yield hydrogen and oxygen from a source such as natural gas or water (Yalcin, 1989). A second method is to use electricity generated by a nuclear reactor to split water by electrolysis. Electrolysis is a well-known commercial process but is subjected to an overall lower efficiency of 24 % (Rosen, 2009). This lack in efficiency is chiefly contributed by the low conversion of heat to electricity (Orhan *et al.*, 2009).

The inefficiency of electrolysis can be overcome by using a thermochemical cycle, compromising a series of chemical reactions with the net reaction of producing hydrogen and oxygen from water. Combining a thermochemical cycle with the heat of a nuclear reactor is one of several processes to produce hydrogen in the future (Orhan *et al.*, 2009). After thermochemical cycles, high temperature water electrolysis is considered to be the next best production method (Rosen, 2009).

Hydrogen from nuclear sources

Three thermal energy sources can be used to supply the heat which will be required for the hydrogen economy: fossil fuels, nuclear power and renewable energy (Rosen, 2009). Currently, 96 % of hydrogen production is achieved with fossil fuels. This approach is expensive, produces large quantities of greenhouse gases and is counterproductive for stimulating a hydrogen economy. Fortunately, new innovative techniques and technologies are currently being developed that result in more affordable, more efficient methods of hydrogen production, lower CO_2 emissions and a lower feedstock cost.

In the past nuclear energy is used to produce electricity. The thermal energy from the nuclear process can be used as an energy source for a thermochemical water splitting cycle for the production of hydrogen and oxygen (Wang *et al.*, 2009). Nuclear energy can provide a significant share of energy on a national scale without contributing to ever growing CO_2 emissions and climate change (Orhan *et al.*, 2009) and it can be utilised for the large-scale use of hydrogen production (Yildez & Kazimi, 2005). This makes nuclear energy the ideal candidate for hydrogen production.

Nuclear technology has been making advances capable of producing reactor coolant with temperatures in the order of 750 °C. The gas turbine modular helium reactor and the High-Temperature gas reactor are potential future high temperature reactor types that could be used to supply high-temperature heat (Wang *et al.*, 2009). Many innovative advances are needed for nuclear-based heat to become a viable practical reality. Nuclear technology has demonstrated the commercial and technological advancement required. It is essential to evaluate these alternative technologies to evaluate their energy efficiencies and cost viability for the production stage (Orhan, Dincer & Rosen, 2008).

The economic viability and efficiency of any alternative system depends highly on the cost of energy and the cost of the technology. Various preliminary cost analyses and alternative routes for nuclear technology found in the report by Yildez and Kazimi (2005) determined that on average long term hydrogen production is driven more cost effectively with nuclear energy than with natural gas (Forsberg, 2003).

Nuclear power can be used for the production of hydrogen mainly in three ways (Yildiz & Kazimi, 2005):

- Using electricity supplied by the nuclear reactor for electrolysis.
- Using a combination of the heat and electricity produced for either high-temperature steam electrolysis or a hybrid process.
- Direct use of the heat for thermochemical processes.

A further advantage of nuclear power is the sustainability of the technology, stable energy supply and flexibility in the size of the production plant (Cilliers, 2010).

Thermochemical cycles combined with a high-temperature cycle have been covered extensively in recent studies. High-temperature heat for hydrogen production is supplied in the form of high-temperature helium which is generated by a high-temperature gas reactor.

Hydrogen market

Worldwide, 50 million tons of hydrogen is consumed per annum. Hydrogen is mainly produced with a large release of carbon dioxide (CO_2), It is therefore not a clean process. In the near future, CO_2 penalties as high as US$30/metric ton of CO_2 will be imposed which will drive up the cost of hydrogen for CO_2 intensive processes such as steam methane reforming.

Currently there are four potential markets for hydrogen: transportation, industrial, electricity and commercial applications in buildings (Cilliers, 2010). Hydrogen has a high energy density and proven production methods that are easy to use. Liquid fuels such as petroleum are currently in the lead for the transportation market but will soon be exhausted (Dopp, 2007). This fact drives the quest of large oil companies as well as motor-vehicle companies such as BMW for a viable alternative energy source. BMW has already built and is currently testing a hydrogen-fuelled concept car as part of the drive to explore alternative fuels (BMW, 2010).

Hydrogen is mainly used in industry for the production of fertilisers, particularly ammonia, and for the reduction of iron ore to produce iron and steel. This process is achieved using syngas, which is a mixture of hydrogen and carbon monoxide (CO). Using syngas lowers the capital cost of the process and is considerably more environmentally friendly than a blast furnace performing the same function. The fertiliser market is not set to increase but it is predicted that syngas usage will grow (Cilliers, 2010).

Syngas is further used for reforming specifically where methane is used in steam reforming to produce syngas for the Fischer-Tropsch reaction. Using clean, non-fossil based hydrogen, the CO_2 outputs can be reduced by 75 % while the coal requirement would be reduced by 40 % which reduces the installed syngas plant cost by 50 % (Chiuta, 2008).

Hydrogen is used in fuel cells to produce electricity. Hydrogen can be used to provide electricity during high demand periods when electricity is expensive. Hydrogen's biggest advantage over electricity is that it can be stored and released on demand and can be supplied to utilities during peak electricity production. Hydrogen with its high energy density also has the potential to be used as a space heater and a source of electricity in buildings.

There is a potentially, significant market for hydrogen which is produced in an environmentally clean manner. In the future, hydrogen will mainly be used as a transportation fuel. A hydrogen network was established in 1999 to develop strategies to introduce a hydrogen fuel structure for Europe. Japan is planning on introducing upwards of 5 million fuel-cell vehicles by 2020
(Wang, Naterer & Gabriel, 2008).

Hydrogen is a light gas with extreme properties. This factor needs consideration in the storage of hydrogen. Pipelines currently being used in the transportation of oil and natural gas are proposed to transport hydrogen (Forsberg, 2003). Hydrogen is generally stored as a liquid where it can be delivered with pumps in its hybrid form. As the lightest element it requires large volumes of storage space for the purpose of driving the hydrogen economy forward.

The disadvantage of its low density increases the cost when hydrogen is used as an energy carrier as more hydrogen will be required to produce the same amount of energy when compared to fossil fuels. Better means of hydrogen storage and energy usage will be required to operate a successful hydrogen economy.

2.2 Physical and thermochemical hydrogen production

Water splitting is achieved in a number of ways such as thermochemical cycles or the pyrolysis of water at 4000 ˚C (Yildez & Kazimi, 2005). Reactors operating at such high temperatures place severe strain on construction materials. The thermochemical cycle bridges this gap by lowering the temperature of thermal decomposition of the water into hydrogen and oxygen. The advantages of using a thermochemical cycle are the low cost of water as the only feedstock, the possibility of achieving up to 50 % efficiency (Rosen, 2009) and the possibility of avoiding CO_2 emissions by using an appropriate heat source such as a high-temperature nuclear reactor.

Over two hundred different thermochemical water splitting cycles have been reported (Wang *et al.*, 2009) with the majority of these operating at a temperature above 850 ˚C (Rosen, 2009). Studies have been done on all the cycles but of these only the sulphur iodine cycle, the HyS process and the CuCl cycle have been reported to be economically viable (Lewis, Masin & O'Hare, 2009).

In the USA, research has been conducted to develop a cycle which delivers hydrogen at a temperature below 550 °C (Rosen, 2009). Lewis, Mason and O'Hare (2008) have done a study to discover the best low temperature thermochemical water splitting cycle for the use of the Canadian super-critical water reactor which has a maximum operating temperature of around 600 ˚C (Naterer *et al.*, 2010). The study concluded that the CuCl cycle was most appropriate for further studies. Other means of hydrogen production are discussed next.

Steam methane reforming

Steam methane reforming is currently the most popular method of hydrogen production. The cycle achieves an 83 % thermal efficiency, works on proven technology, produces hydrogen gas at a cost of around US$0.75/kg, depending on the cost of natural gas, and is currently the most economical option to produce hydrogen (Cilliers, 2010). The syngas produced by this method is used in the

Fischer-Tropsch reactor with hydrogen to produce long carbon chains and into oil. The steam-methane reforming process is not CO_2-emission free and its feedstock is natural gas whose price fluctuates on a regular basis.

Additional methods of hydrogen production from fossil-based sources are the partial oxidation or auto-thermal reforming of methane, coal gasification and biomass pyrolysis (TTcorp, 2011).

The steam reforming-process entails three chemical steps as shown below (Kemp, 2008):

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

$$CH_4 + 2H_2O \leftrightarrow CO_2 + 4H_2 \qquad \Delta H = +165 \text{ kJ/mol} \qquad (2)$$

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

Methane gas is fed with steam to produce carbon monoxide (CO), CO_2 and hydrogen. Hydrogen is subjected to a purification process to be delivered at a desired quality. CO is reacted further with steam to produce CO_2 and hydrogen, known as the water-gas-shift reaction, to obtain the desired mix of hydrogen and CO for the Fischer-Tropsch reactor (Kemp 2008).

Sasol in South Africa produce oil from coal and natural gas by using the Fischer-Tropsch process. The process results in Sasol becoming one of the most polluted CO_2 sectors in the world (IEA, 2011). The water-gas shift reaction can be avoided by combining a nuclear reactor and a thermochemical cycle, which would result in a 75 % reduction of the total CO_2 emissions (Chiuta, 2008)

Electrolysis

Electrolysis is the electrical dissociation of water into hydrogen and oxygen. It is a commercially proven technology and the electrical energy can come from renewable or non-renewable sources. Industrial electrolysis processes have an efficiency rating between 45 % and 55 % with hydrogen produced at roughly US$1.95/kg (Cilliers, 2010).

With a production rate between 10 and 20 tons/day, off-peak electrolysis has an overall lower production cost for hydrogen (Naterer *et al.*, 2010). Thus during low peak periods when electricity is at its lowest price, electrolysis is used more economically than thermochemical cycles to produce hydrogen.

The dissociation of water is achieved by applying an electric potential over a cell through water. Water is the feedstock and electricity is the energy source. Each cell consists of a cathode (where hydrogen is formed), an anode (where oxygen is formed) and a conducting medium such as a salt bridge.

The half-cell reactions for alkaline cells are (Dopp, 2007):

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

Anode: $2OH^- \leftrightarrow 0.5O_2 + H_2O + 2e^-$

Net reaction: $H_2O \leftrightarrow H_2 + 0.5O_2$

The reaction rate for electrolysis is determined by the cell voltage. Electrolysis requires a theoretical cell voltage of 1.23 V over the cell; however with this low voltage the reaction rate is too slow to use commercially. Higher voltages are used to achieve higher reaction rates, however using this approach leads to lower efficiency as energy is lost as heat (Dopp, 2007).

Various methods have been applied to improve the overall efficiency of this process. Methods include increased pressure and temperature and the introduction of a catalyst. A recent study on electrolysis has replaced graphite electrodes with carbon nanotubes and found that hydrogen production has doubled (Dubey *et al.*, 2010).

High-temperature steam electrolysis (HTSE) can be used with good overall efficiency. HTSE is the electrolysis of steam at high temperatures and is widely considered to be a more efficient and environmentally friendly way of producing hydrogen. As higher operating temperatures often yield better energy efficiency and better power conversion, the HTSE is advantageous when combined with a high-temperature reactor with a more efficient power cycle (Yildez & Kazimi, 2005).

Sulphur iodine

The sulphur-iodine process is a thermochemical cycle, producing oxygen and hydrogen from the feedstock water and high-temperature heat. The chemical reactions in the cycle are shown below:

$I_2 + SO_2 + 2H_2O \leftrightarrow 2HI + H_2SO_4$ (< 120 °C) $\Delta H = -216$ kJ/mol

$H_2SO_4 \leftrightarrow SO_2 + H_2O + 0.5O_2$ (> 800 °C) $\Delta H = +371$ kJ/mol

$2HI \leftrightarrow H_2 + I_2$ (> 300 °C) $\Delta H = + 12$kJ/mol

The cycle is a closed-loop cycle with no harmful emissions or by-products. The maximum temperature of the cycle is greater than 800 °C (Wang *et al*., 2010)

Such high temperatures limit the number of possible heat sources. Possible nuclear reactor types are heavy metal reactors, molten salt or the PBMR - helium cooled high temperature reactor which delivers heat between 850 °C and 900 °C.

Sulphur Hybrid (HyS) cycle

The HyS is a thermo-chemical water splitting cycle, decomposing water into hydrogen and oxygen. The cycle has been extensively studied at North-West University for a number of years. The chemical reaction steps are shown below (Chiuta, 2008):

$H_2SO_4 \leftrightarrow H_2O + SO_3$ (Thermal decomposition > 300 °C)

$SO_3 \leftrightarrow SO_2 + 0.5O_2$ (Thermal decomposition, 870 °C)

$2H_2O + SO_2 \leftrightarrow H_2SO_4 + H_2$ (Electrolysis, 100 °C – 120 °C)

Heat from the nuclear reactor coolant is used as an energy source for the cycle. Proton exchange membranes are used in the electrolyser. At the anode, sulphur dioxide and water are oxidised to produce protons and sulphuric acid. The protons diffuse through the membrane to the cathode and are reduced by the electrons to produce hydrogen gas.

The HyS process operates at a pressure of 86 bar with an operating temperature of 1143 °K and an overall efficiency of 35.3 % (LHV), a thermal efficiency of 35.5 % and an SO_3 conversion of 75 % by lowering the pressure to 3 bar (Cilliers, 2010). The cycle produces no harmful emissions or by-products. It is proposed that a helium-cooled high-temperature PBMR should be used as the heating source.

2.3 The copper-chloride (CuCl) cycle

Description

The copper-chloride (CuCl) cycle consists of a number of chemical reactions, one of which requires electrical energy, which results in the splitting water into hydrogen and oxygen. The chemical reactions involve intermediary copper and chlorine products which are recycled in a closed loop. Only water (H_2O), high-temperature heat, derived from a high-temperature nuclear reactor such as a PBMR, and electricity is fed into various reactors. Hydrogen and oxygen are produced with no emissions or by-products released to the environment (Orhan *et al.*, 2008).

The CuCl cycle was identified by the Argonne National laboratory (ANL) as a highly promising cycle for the thermochemical splitting of water. This cycle can potentially be coupled to the Canadian Supercritical Water Reactor (SCWR). Argonne national Laboratories and the University of Ontario Institute of Technology have developed enabling technologies for this cycle (Rosen, 2009). The majority of this mini-dissertation's literature survey derives from research produced from these facilities.

The CuCl cycle is considered promising for the following reasons
(Serban *et al*., 2004):

- The maximum temperature of the cycle is less than 550 ˚C. The lower temperature, compared to the HyS process, enables the use of multiple proven heat sources.
- The intermediate chemicals are relatively safer, inexpensive and more abundant than the HyS process.
- With appropriate steps, minimal solids handling is necessary.
- All reactions have been proven in the laboratory.

The biggest disadvantage is the electrochemical step. Historically an electrochemical step imposes significant cost; however the CuCl cycle's electrical potential requirements are lower than those of direct water electrolysis.

The CuCl cycle consists of five interconnected reaction vessels combined with several heat exchangers. The CuCl cycle’s chemical reaction steps are shown below:

Step 1: $2Cu(s) + 2HCl(g) \rightarrow H_2(g) + 2CuCl(s)$	Exothermic, 430 ˚C → 475 ˚C
Step 2: $2CuCl(s) \rightarrow CuCl_2(aq) + Cu(s)$	Electrolysis
Step 3: $CuCl_2(aq) \rightarrow CuCl_2(s)$	Drying step
Step 4: $2CuCl_2 + H_2O(g) \rightarrow CuO.CuCl_2 + 2HCl(g)$	Endothermic, 400 ˚C
Step 5: $Cu_2OCl_2(s) \rightarrow 2CuCl(\mathit{l}) + \frac{1}{2}O_2(g)$	Endothermic, 530 ˚C

Step 1 is the chemical reaction where hydrogen production takes place. Copper (Cu) particles enter along an inclined bed to be melted. Hydrogen chloride (HCl) gas enters and passes through the chamber. CuCl and hydrogen gas are produced. The reaction is exothermic (Rosen, 2009).

Step 2 is the electrolyser step. CuCl(s) enters and Cu particles and copper dichloride ($CuCl_2$) are produced in an electrochemical cell.

Step 3 is where $CuCl_2$ is dried. Aqueous $CuCl_2$ exits from the electrochemical cell. The mixture is dried to produce solid $CuCl_2$ required for step 4 (Rosen, 2009).

Step 4, involves a chemical reaction known as the hydrolysis step. HCl is produced when high-temperature steam at 400 °C and solid $CuCl_2$ are mixed to produce two exit flows. One exit stream contains HCl and the copper oxychloride ($CuO.CuCl_2$) (Rosen, 2009).

Step 5 is a chemical reaction where oxygen is generated. This is the highest temperature in the process and takes place at a temperature of around 530 °C. $CuO.CuCl_2$ enters the reactor where it is thermally dissociated into oxygen (O_2) and CuCl (Rosen, 2009).

The CuCl cycle has challenges associated with each step:

- Step 1: More efficient performance in the mixing chamber and better understanding of the particle mixing needs to be catered for (Rosen, 2009).
- Step 2: Requires heat exchangers which can operate and process fluids in extreme operating conditions. AECL investigated combining step 1 and step 2 to reduce the challenges of solids handling by using direct electrolysis of HCl and CuCl to produce hydrogen. The chemical reaction is shown below (Dokiya & Kotera, 1976):

$$2CuCl(aq) + 2HCl(ag) \rightarrow H_2(g) + 2CuCl_2(aq)$$

- Step 3 is the drying step which can be very energy intensive. Improved evaporator efficiency and methods of waste heat utilisation are required (Rosen, 2009).
- Step 4: excess water is needed and a reduction in the amount of water is required.
- Step 4 and step 5: Better understanding is required of the solubility of $CuCl_2$ and of $CuO.CuCl_2$ in a mixture of steam and HCl (Rosen, 2009).
- Solids handling and corrosive working fluids presents unique challenges (Naterer *et al.*, 2010).

The biggest advantage of CuCl is the lower temperature requirement of 530 ˚C for the cycle when compared to 900 °C for the hybrid sulphur and sulphur Iodine process. The lower temperature lowers the cost of materials, enables the use of low-grade waste heat, reduces the thermal burden and the demands made on the construction materials, improves heat demand and management and flexibility in reactor type (Lewis, Mason & Vilim, 2005). Other advantages include lower voltage requirements, common chemical agents and reactions which go to completion without side reactions (Naterer *et al.*, 2010). Cost analysis has shown that production cost of the SI-cycle and the CuCl cycle are similar ie. fall within the same range (Wang *et al.*, 2009).

Combining a low- temperature cycle with a high-temperature reactor presents the opportunity for co-generation which results in significantly higher closed-cycle efficiencies (Orhan, Dincer & Rosen, 2009). Transferring heat between the various endothermic and exothermic reactions through the use of heat exchangers is crucial for achieving high thermal efficiency (Jaber, Naterer & Dincer, 2010).

Waste heat is produced within the cycle. One unique advantage of the CuCl cycle is the ability to utilise low-grade heat with one such process step being the drying step. Waste heat which would have otherwise been rejected to the environment can now be utilised at minimal or no cost while improving the overall economics of the cycle (Naterer *et al.*, 2010). Waste heat can be further advanced by using a heat pump (Rosen, 2009).

4-step vs 5-step process

In the 5-step cycle, Cu is produced electrolytically and then moved to the exothermic reactor where it is reacted with HCl to produce CuCl and hydrogen gas (Naterer *et al.,* 2010). Step 1 consists of molten CuCl, HCl and H_2 at high temperature which is considered to be a very corrosive working environment requiring a large amount of solids work, the CuCl and $CuCl_2$ (Wang *et al.*, 2009). A new reaction eliminates these problems has been proposed by Dokiya & Kotera (1976).

Atomic Energy of Canada Limited (AECL) is currently investigating a reaction step where CuCl is electrochemically reacted with HCl to produce hydrogen directly (Jaber, Naterer & Dincer, 2010). The reaction with the heat of reaction is shown below (Magali *et al.*, 2010):

$$2CuCl(aq) + 2HCl(aq) \rightarrow H_2(g) + 2CuCl_2(aq). \qquad \Delta H = +93.76 \text{ kJ/mol } H_2$$

The 4-step cycle combines steps 1 and 2, thereby eliminating the intermediate production step and the handling needed for the Cu solids (Naterer *et al.,* 2010).

Advantages of the new cycle are the milder working conditions, greatly reducing the equipment, material and solids handling challenges. Overall it was found that the heat requirements of the new cycle are not significantly different from the 5-step cycle, and that the overall efficiencies of the two cycles fall within the same range, between 37 % and 54 %, depending on the amount of heat recovered (Wang *et al.*, 2009).

The reaction takes place in an aqueous solution of HCl, reducing the complexity of separating water and HCl after the hydrolysis step. By increasing HCl in the feed to step 4, where it is a product, decreases the equilibrium conversion due to azeotrope formation, making it more difficult to obtain either pure water or pure HCl (Masin & Lewis, 2005). Using a mixture of HCl and water saves excess separation energy losses. Disadvantages of this step are potentially adverse dependence on current and voltage on the concentrations of reactants and products (Wang *et al.,* 2009). This mini-dissertation will be predicated on the 4-step cycle.

New proposed CuCl cycle

A new cycle developed and reported by Wang *et al* (2009) compromising the following chemical reactions:

1) $2CuCl(aq) + 2HCl(aq) \rightarrow 2CuCl_2(aq) + H_2(g)$	Electrolysis at 30 ˚C → 80 ˚C
2) $2CuCl_2(aq) + 4H_2O(free) \rightarrow 2[CuCl_2 \bullet 2H_2O]$ (slurry)	70 ˚C → 30 °C
3) $2[CuCl_2 \bullet 2H_2O](sl) \rightarrow 2CuOHCl(s) + 2HCl(g) + 2H_2O(g)$	150 °C with fast HCl removal
4) $2CuOHCl(s) \rightarrow CuCl_2(s) + CuO(s) + H_2O(g)$	285 ˚C
5) $CuO(s) + CuCl_2(s) \rightarrow 2CuCl(molten) + \frac{1}{2}O_2(g)$	530 ˚C

The advantage of this cycle is its greatly reduced use of excess water as a result of the fast removal of HCl, in step 3. A number of reactions are very similar to the 4-step cycle and similar technology on these reactors can be used, including the heat transfer techniques developed for the 4-step cycle.

The cycle’s biggest potential challenge is the chemical properties and the relatively unknown chemical reactions. A number of these chemicals are relatively unknown with very little data being available on the chemical or their reactions. Nevertheless, the new cycle should be investigated since it has the potential to be more economically viable and thermally efficient than the current 4-step cycle.

2.4 CuCl cycle reactors

In this section each of the reactors will be described and information gathered from literature will be summarised and presented.

Electrolyser

The electrolyser's chemical reaction step is shown below:

$$\mathbf{2CuCl(s) + 2HCl(aq) \rightarrow H_2(g) + 2CuCl_2(aq)}$$

AECL is currently investigating proposed modifications to the CuCl cycle. The electrolyser is potentially the most expensive reactor in the cycle because of the use of electricity (Orhan, Dincer & Rosen, 2009). AECL has successfully demonstrated this step and have produced hydrogen for several days with the CuCl/HCl electrolyser (Ferrandon *et al.,* 2009).

The following challenges have to be addressed to operate the electrolyser (Lewis, Masin & Vilim, 2005):

- The design of the electrochemical cell
- Identification of a suitable membrane
- Operating parameters

The electrolysis requires an HCl concentration of at least 11 M and a minimum of 6 M. Any lower than 11 M and copper metal deposits will begin to form at a current density of 0.1 A/cm^2 (Naterer *et al.,* 2010). The conductivity of the cell reaches a maximum at 6 M HCl thus a too high concentration is also not indicated (Stolberg *et al.,* 2008). The concentration of the CuCl mixture is 1 M (Stolberg *et al.,* 2008); however a lower concentration is preferred. Solid $CuCl_2$ will be exiting via a conveyor belt (Rosen, 2009). Hydrogen production was observed with potentials as low as 0.5 V however the best results were obtained around 0.65 V (Naterer *et al.,* 2010).

The electrolyser should ideally be operated at a high temperature and pressure. AECL found the optimum conditions to be a pressure of 24 bar and a temperature range of 70 ˚C to 80 ˚C. The pressure further assists with storing hydrogen gas at a pressure of 300 psi (Ferrandon *et al.*, 2008). The free energy for the electrochemical cell is positive so energy will be needed for the reaction to proceed (Naterer *et al.*, 2010).

AECL has determined the following parameters for the electrolyser:

- Current density of 0.1 A/cm^2 (Naterer *et al.*, 2010)
- Cell voltage of between 0.6 V and 0.7 V (Naterer *et al.*, 2010)
- Reversible cell potential is -1.23 V (Naterer *et al.*, 2010)
- Potentially 75 % conversion. (Naterer *et al.*, 2010)
- Preferred operating concentration is 0.5 M CuCl and 11 M HCl (Naterer *et al.*, 2010)
- ΔH = 93.76 kJ/mol (Magali *et al.*, 2010)

The data available at present are insufficient to allow a comprehensive analysis on the electrolyser. The energy requirements of the electrolyser will be calculated in the manner adopted by Cilliers (2010) in the study of the HyS cycle. Only the inlet and outlet compositions and the assumed voltage and current values will be used (Lewis *et al.*, 2008).

The reaction rate for the CuCl/HCl electrolysis improves with increased temperature and CuCl concentration (Naterer *et al.*, 2010). The current density is higher for a given cell emf at 80 ˚C than at 25 ˚C (Naterer *et al.*, 2009). The electrolysis efficiency is defined as the voltage efficiency multiplied by the current efficiency (Naterer *et al.*, 2010).

The anode feed tank contains the feedwater and the CuCl and makeup HCl will be added to keep the CuCl dissolved (Lewis *et al.,* 2008). Silver refining equipment will be used to remove the $CuCl_2$ product (Rosen, 2009). The electrolyser requires a membrane to prevent copper species from crossing over to the cathode side as copper can act as a poison to the electrodes (Naterer *et al.*, 2010).

The electrodes used in the past usually consisted either of solid platinum or glass. For the CuCl/HCl electrolyser the difference between the glass electrode and the platinum electrode can be greatly reduced at higher pH levels. The difference is more comprehensive at all pH levels when using a high surface area carbon black electrode, which makes carbon black surfaces a cheaper and more appealing electrode for the electrolyser (Ranganathan & Easton, 2000).

Carbon nanotubes were recently introduced as an electrode for water electrolysis. Their high efficiency as an electrode needs to be further investigated with a view to improving the electrolyser performance (Dubey *et al.*, 2010).

Calculating the energy required for the electrolyser is done according to the precedent set by Cilliers (2010). The electrical power requirement of the electrolyser is calculated using the operating cell voltage and the current density. To calculate the power used for the electrolyser, the cell voltage has to be determined by first determining the acidic concentration of HCl, the amount of CuCl which is dissolved and the reversible potential. The cell voltage for this study has been reported in literature as 0.65 V (Naterer *et al*., 2010).

The required amount of electrical power is calculated by multiplying the voltage and the current values. The current is calculated by the use of Faraday's law. Faraday's first law states that the quantity of a substance produced by electrolysis is proportional to the quantity of electricity used.

The calculation of the quantity of energy which will be required begins with Faraday's constant which is the quantity of charge carried by one mole of electrons:

$$F = N_A \bullet \text{charge of electron} \qquad (1)$$

$$F = 6.022\text{x}10^{23}\ \text{mol}^{-1} \bullet 1.602192\text{x}10^{-19}\ \text{C} \qquad (2)$$

The amount of energy carried by one electron is calculated. The energy required to transfer, F, a number of electrons will be multiplied by the number of electrons exchanged, n(e). This gives the amount of current flowing through the cell, Q:

$$Q = n(e) \times F \tag{3}$$

To finally calculate the power requirement, the current is multiplied by the voltage

$$E = Q \times V \tag{4}$$

Dryer

The following process takes place in the dryer:

$$\mathbf{CuCl_2(aq) \leftrightarrow CuCl_2(s)}$$

The dryer is used to remove any excess water from the $CuCl_2$ which comes from the electrolyser. Even though the following reactor, step 3, does use steam, it was found to be more thermally efficient to separate the hydrolysis and the drying processes (Naterer *et al.*, 2010), 1.1 mole of H_2O must be evaporated to obtain 1 mol of dry solid $CuCl_2$ (Naterer *et al.*, 2008). When a comparison was performed by Wang *et al.* (2010), it was assumed that the energy required for the dryer was 122 kJ/mol H_2. The heat that must be added to ensure that the water evaporates (Naterer *et al.,* 2009) makes drying one of the most energy-intensive steps in the whole process.

Large inefficiencies occur when high-grade heat is used in the drying process. Preliminary calculations show that in combination with some shaft work, large quantities of water are removed at a temperature of 70 ˚C. Drying can be effective at a temperature as low as 35 ˚C, but this low temperature is not recommended as the quality of the product will diminish (Naterer *et al.*, 2009).

Waste heat can be supplied at the required temperatures and is currently being investigated. The use of waste heat is particularly attractive when the cycle is used in combination with a high-temperature gas reactor as more than half of an high-temperature reactor loses its energy as waste heat (Lewis, Masin & Vilim, 2005). Waste heat is available at around 90 ˚C.

Forty percent of the heat produced for electricity is converted to electricity, thus the other sixty percent can be utilised as waste heat (Naterer *et al.,* 2008). The waste heat can be further utilised to supply more heat by using heat pumps. High coefficients of performance have been predicted for direct-contact heat exchangers with internal heat recovery and a CuCl heat pump (Naterer *et al.*, 2010).

Spray drying is a new improved drying method which is considered for the efficient removal of water as the spray droplets have a large surface area, provided the liquid atomises into sufficiently small droplets (Naterer *et al.*, 2010). Further studies have shown that considerable drying can occur through the difference in humidity alone (Naterer *et al.,* 2008).

The cycle's overall efficiency is also improved by drying the slurry rather than an aqueous solution (Naterer *et al.*, 2009). Dewatering by means of gravity, filtration and sedimentation is also used (Naterer *et al.*, 2008a) to reduce the mixture to slurry. The benefit of flash drying has been shown to be negligible (Naterer *et al.,* 2008b).

Hydrolysis Reactor

The hydrolysis reaction is shown below:

$$2CuCl_2(s) + H_2O(g) \rightarrow 2HCl(g) + CuO.CuCl_2(s)$$

The hydrolysis reaction is the least understood in the CuCl cycle, but it is crucial for the purpose of determining whether or not hydrogen can be produced cost-effectively (Masin & Lewis, 2005). The reaction has been proven at Argonne National Laboratory (Ferrandon *et al.*, 2009) and several challenges have been identified accordingly that will require specific determinations (Lewis, Masin & Vilim, 2005):

- Conditions that will inhibit the formation of CuCl and chlorine
- Minimum amount of steam required for a complete reaction
- The optimum temperature that will provide suitable kinetics while still enabling mating with the other reactions

The hydrolysis reaction is considered to be among the most challenging steps for two reason, the competing reaction of $CuCl_2$ thermally decomposing into CuCl and chlorine gas and a high demand for excess steam (Ferrandon *et al.*, sa). The required inhibition of chlorine formation can be achieved by ensuring that the hydrolysis reaction is run as close to 100 % as possible
(Lewis, Masin & O'Hare, 2009).

The CuCl cycle can become an efficient low-cost process if it can reduce excess water consumption (Naterer *et al.*, 2010). The hydrolysis reaction is not easily controlled to full reaction without the use of excess steam; and besides at a temperature of 400 °C the HCl gas may also react with common metal as well as their protective oxide films (Naterer *et al.*, 2008a).

To reduce the excess steam requirements for the production of $CuO.CuCl_2$, the reactor is operated at a lower pressure of 0.5 bar (Wang, Naterer & Gabriel, 2008). The lower pressure reduces the steam to $CuCl_2$ molar ratio of 17 to 12 at 0.5 bar (Naterer *et al.*, 2010). The drop in pressure reduces the demand for costly steam which decreases capital cost and energy usage (Ferrandon *et al.*, 2008).

The reaction is an endothermic non-catalytic solid-gas reaction operating between 350 °C and 400 °C (Naterer *et al.*, 2008a). Studies on the reactor have determined that at a pressure 0.5 bar and a water-to-$CuCl_2$ molar ratio of 12, a 100 % conversion is achievable at 370 °C, (Naterer *et al.*, 2010). The hydrolysis reaction has a relatively short residence time of 5 s (Ferrandon *et al.*, sa) and the reaction rate of the hydrolysis reaction is 2 to 2.5 times slower at 300 °C than at 350 °C (Lewis, Masin & Vilim, 2005). Operating at higher temperatures is not recommended as chlorine will start to form above 390 °C (Forsberg, 2003), reaching a peak at 460 °C (Ferrandon *et al.*, 2009).

Decomposition Reactor

The following decomposition reaction takes place at 530 ˚C (Naterer *et al.*, 2010):

$$\mathbf{CuO.CuCl_2\,(s) \rightarrow 2CuCl\,(molten) + \frac{1}{2}O_2\,(g)}$$

$CuO.CuCl_2$ enters the reactor at 430 °C where it is thermally decomposed into oxygen and molten CuCl at a temperature above 500 ˚C (Naterer *et al.,* 2008a). The reaction is endothermic and requires the highest temperature of the cycle (Lewis, Masin & Vilim, 2005).

Oxygen is evolved at temperatures ranging from 450 ˚C to 530 ˚C. In bench scale experiments all the oxygen was recovered at a temperature of 530 ˚C (Ferrandon *et al.,* sa).The activation energy of 50 kJ/mol suggests that a catalyst is not required and an average sized reactor can be used (Lewis, Masin & Vilim, 2005). The reaction is relatively simple with no side reactions (Lewis *et al.,* 2008) and has a typical residence time of 60 min (Ferrandon *et al.*, sa).

$CuO.CuCl_2$ will not melt in the CuCl as it is first decomposed at 470 ˚C. A side reaction can occur if residual $CuCl_2$ is present as shown below (Naterer *et al.*, 2010):

$$2CuCl_2 \rightarrow 2CuCl + Cl_2$$

Significant amounts of chlorine must be avoided in this reaction if it occurs with the minimum amount of $CuCl_2$ present in the decomposition reactor. The most effective method of removing the CuCl is to ensure that the hydrolysis reaction is run as close to completion as possible (Naterer *et al.*, 2008a).

Heat is transferred from the molten CuCl to the $CuO.CuCl_2$. The molten bath can be sustained by the reaction product itself. The reactor is heated from the wall with a double-shell structure without the use of electricity. The construction material must be resistant to high-temperature oxygen, CuCl and HCl and an operating temperature of 530 ˚C is recommended (Naterer *et al.*, 2008a). The operation will be safest if the lowest feeding temperature is above 430 ˚C, bubbles will begin to form if particles enter the reactor at a temperature above 430 ˚C (Naterer *et al.,* 2009).

Heat recovery is an ongoing study applicable to the CuCl cycle. Full heat recovery can be achieved by removing heat from CuCl with air in a direct-flow, counter-current heat exchanger (Jaber, Naterer & Dincer, 2010). Heat can also be recovered from oxygen; however with the increase in heat the volume of oxygen will be three times greater (Naterer *et al.*, 2008a).

3. Proposed CuCl Cycle

The literature proposed various methods for the production of hydrogen explaining the physical properties and potential uses of hydrogen. Additional theory for various thermochemical cycles was presented including the CuCl cycle. Additional theory for the CuCl cycle is presented here in order to present the working conditions that will be matched in simulation.

The CuCl cycle model is presented as a flow sheet. The flow sheet package used for this model is Honeywell's Unisim^{TM}. The fluid package selected for this model is Peng-Robinson. It's noted the 4-step reaction mechanism will be modelled in this mini-dissertation.

Twice the amount of water that is stoichiometrically required is used in all but two of the models. The correct amount of steam is used in these models.

Four main models will be presented here with three additional models with variations presented at a later stage. First is the Base model in which no heat exchange takes place between intermediary streams. Further models will include heat-exchange networks that will attempt to optimise the process. The second model, the Canadian model, is based on the heat-exchange network developed in Canada. Thirdly the Kemp model presents the author's own heat-exchange network design. The fourth is the Excess model which includes the need for excess steam in the hydrolysis reactor and is developed from the Kemp model.

When looking at the models a symbol with an "S" is seen. Unisim^{TM} has a function, called a "set" function, where a stream value can be set as a multiple of another. This function is seen on the model as it was used to continuously obtain the correct amount of mass in the feed streams. The symbols are left on the models to help assist individuals studying this mini-dissertation and who wishes to copy the models.

Water is stoichiometrically fed to the cycle on a mole basis of 1:1 with hydrogen; however additional water always enters the cycle. Wherever possible the inlet water stream is split to provide one stream with a stoichiometrically correct number of moles of water while another stream supplies any additional water. The set function described above sets the number of moles in the feed streams to a stoichiometric amount based on the water feed stream, allowing the user to only change one value and having all the other values correct themselves. This technique was particularly useful when scaling up.

3.1 Base Model

The equations of the CuCl cycle are repeated below:

Step 1: $2CuCl(aq) + 2HCl(aq) \rightarrow H_2(g) + 2CuCl_2(aq)$. Electrolyser

Step 2: $CuCl_2(aq) \rightarrow CuCl_2(s)$ Drying step

Step 3: $2CuCl_2 + H_2O(g) \rightarrow CuO.CuCl_2 + 2HCl(g)$ Endothermic, 400 ˚C

Step 4: $Cu_2OCl_2(s) \rightarrow 2CuCl(l) + ½O_2(g)$ Endothermic, 530 ˚C

The basic flowsheet is shown in figure A-1, pg 91. All the models are developed from the Base model. For the first three models it is assumed that the steam is double the stoichiometric value.

Working from left to right in figure A-1, an aqueous mixture of hydrochloric acid (HCl) is fed to the cathode of the electrolyser, CRV-100, and an aqueous mixture of copper chloride is fed to the anode of the electrolyser. The electrolyser is viewed as a black box where the reaction (step 1) taking place there produces hydrogen (H_2) gas and an aqueous mixture of cupric chloride ($CuCl_2$).

It is assumed that the electrolyser functions at 75 % efficiency, that any un-reacted reagents, such as HCl, are recycled and only the products leave the electrolyser in the exit streams. For the purpose of this mini-dissertation, CRV-100, is deemed to have a 100 % conversion rate to make the model easier to follow. The amount of electricity consumed is proportional to the amount of hydrogen produced. Electricity for the electrolyser is generated from the hot helium supplied by the nuclear reactor. The conversion of heat to electricity is assumed to be 40 %.

The $CuCl_2$ is dried to a slurry by means of filtration and gravity before entering the dryer. These processes do not require thermal energy and will not be simulated. The slurry of $CuCl_2$ enters the dryer where all the water is removed. The dryer, V-100, incorporates flash drying and spray drying with the latter having been shown to be the most effective (Naterer *et al.*, 2010). The heat required for the drying process is provided by the waste heat generated from the production of electricity and from other material streams which still have enough low-quality heat available.

Dried $CuCl_2$ is heated to a temperature of 370 °C with the heat source E-106, and is then fed to the hydrolysis reactor, CRV-101. Water under atmospheric conditions is heated to 400 °C using the heat source E-100. The hydrolysis reactor is heated directly by the hot helium and operates at a pressure of 0.5 bar and a temperature of 370 °C.

The HCl/water mixture leaves the reactor as a gas and the copper oxychloride ($CuO.CuCl_2$) leaves as a solid. The HCl/water mixture is cooled to a liquid using the coolant source E-101 and then pumped to 24 bar for the electrolyser using pump P-100. The mixture is an aqueous solution to facilitate the electrolyser and the pump.

The HCl/water mixture is supercooled for the simulation to -95 °C with imaginary coolant source E-107 to provide a liquid for the pump. This imaginary supercooler is placed to trick Unisim^{TM} to provide the electrical energy required for the pump. The energy input value for cooling source E-107 is not considered a part of the simulation nor the energy balance.

The $CuO.CuCl_2$ is heated to a maximum temperature of 430 °C in the heat source E-111 to prevent the formation of bubbles and to prevent decomposition. The heated $CuO.CuCl_2$ is sent to the decomposition reactor, CRV -102, where it is decomposed into CuCl and Oxygen (O_2) at 530 °C. The decomposition reactor is heated by the hot helium.

The main heat source for each model is the hot helium supplied by the nuclear reactor at 750 °C and returned at 300 °C while delivering 350 MW of thermal heat. Each of the following three models has a different method of exchanging the heat of the intermediary streams to achieve the best possible heat-exchange network.

Assumptions

Unisim^{TM} has its own way of representing the reactors and electrolysers and in performing calculations on its models. In order to work more effectively with Unisim^{TM} the following assumptions were made while developing the models:

- The Base case, the Canadian and the majority of the Kemp models are treated as stoichiometric models. All three models will have stoichiometric amounts of CuCl and HCl fed in. This is not the correct amount for the final model which will be used when a pilot plant is developed. The amount of water is double the stoichiometric amount. The excess water required for the hydrolysis reactor is considered to be separate from these models and is modelled in the Excess model and in a variation of the Kemp model.
- Except for the excess model, one mole of water for every two moles of HCl is fed to the electrolyser to assist the modelling of the dryer.
- The HCl/water mixture and the molten CuCl stream are not recycled in the model; however they are identical to the feed streams which run into the electrolyser. The recycle stream adds complexity to the model while values are adjusted, making it more difficult to work with the models.
- The water fed to the electrolyser does not have to be the correct amount as water does not react in the electrolyser, it will be removed in the dryer by a heat source and for stoichiometric models will be unnecessary. In all the models the dryer uses waste heat and is always in excess, thus it will not be shown.
- A number of energy streams labelled “QNA” do not form part of the energy balance as their energy values are calculated in Excel^{TM} and placed elsewhere in the model or they are used to obtain an imaginary product such as liquid HCl.
- Solid CuO.CuCl2 and solid CuCl cannot be pumped and as such will presumably reach the required pressure by other means than pumping.

3.2 Canadian Model

This stoichiometric model is based on figure 3-1 (Naterer et al., 2010) shown below.

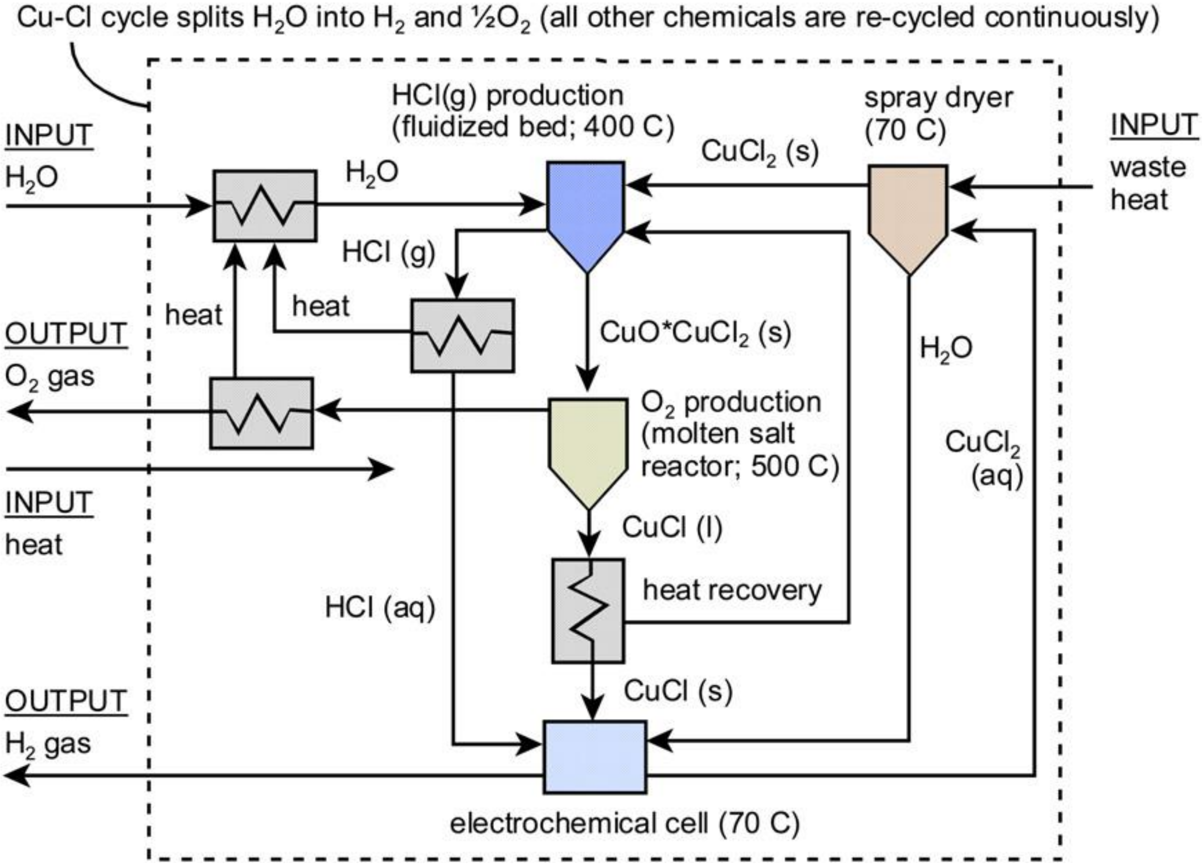

Figure 3-1: Schematic of the Canadian CuCl cycle (Naterer et al., 2010)

A flowsheet developed in Unisim^{TM}, based on figure 3-1, is shown in figure A-2 pg 92. Only the heat-exchanger network differs from the Base model.

The Canadian heat-exchanger network prioritises the heating of the hydrolysing reactor. Molten CuCl, leaving the decomposition reactor at 530 °C, is cooled to 70 °C in heat exchanger E-104 with air and is sent back to the electrolyser. The heat which is recovered is used to heat the hydrolysis reactor. Water enters in stream 9 and is heated by the oxygen exiting the decomposition reactor at 530 ˚C in heat exchanger E-103. The hydrochloric acid heats the water in heat exchanger E-101 where afterwards the HCl/water mixture is recycled back to the electrolyser. Water is finally heated to 400 °C with heat source E-100.

In figure 3-1, neither the $CuCl_2$ nor the $CuO.CuCl_2$ is heated. Air is used as a heat transfer medium to transfer heat from the molten CuCl throughout the process. After using the air to heat the hydrolysis reactor, it is used to heat the $CuCl_2$ in heat exchanger E-106. Helium will be used to heat the $CuO.CuCl_2$, as it is the only medium with a high enough temperature to heat $CuO.CuCl_2$ to its desired temperature.

Ferrandon *et al.* (sa) built an Aspen^{TM} model which supplied excess steam at a ratio of steam to $CuCl_2$ of 17 on a mol basis as shown in figure 3-2. Water from the crystalliser, water from the electrolyser and CuCl at 366 °C is mixed together and sent to the anode side of the electrolyser. No cooling source is seen for the water at 366 °C. Water leaving from the cathode side of the electrolyser to the hydrolysis reactor is heated by cooling HCl gas from the hydrolyser and by the cooling of molten CuCl from the decomposition reactor. Heating of $CuO.CuCl_2$ is achieved by the decomposition reactor. Oxygen is used to preheat the $CuCl_2$ to be dried at 150 °C. The mass and energy balances are shown in tables A-8 and A-9, pg 145.

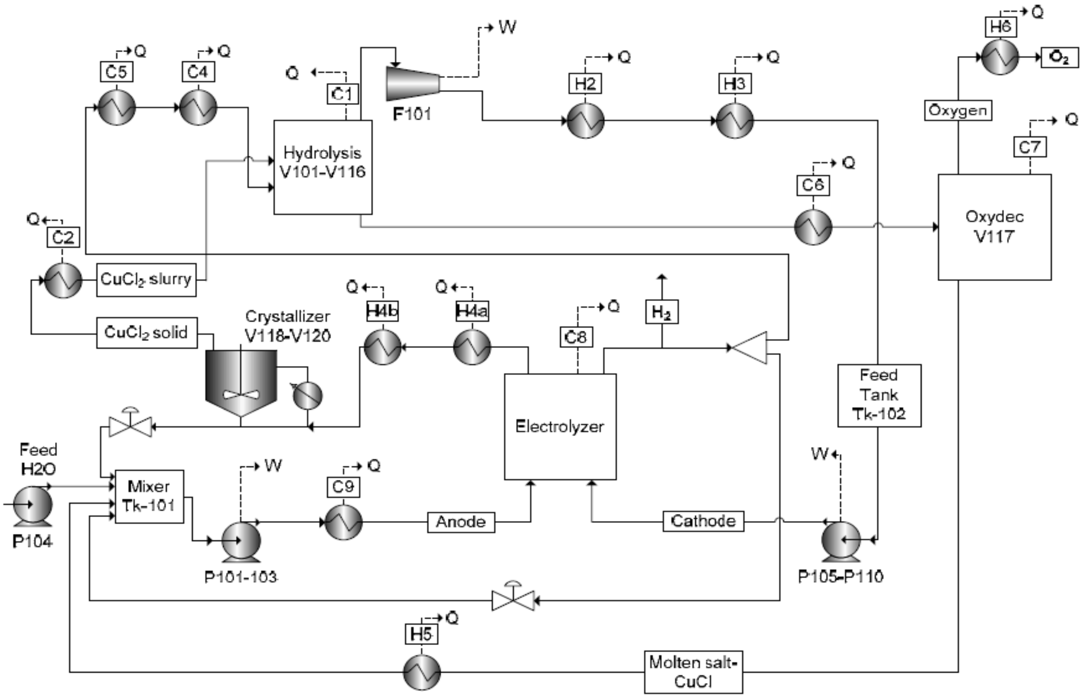

Figure 3-2: Aspen flowsheet of the Canadian model with excess steam (Ferrandon et al., sa).

3.3 Kemp model

The Kemp model differs from the Canadian model. Emphasis is placed on heating the excess water with molten CuCl using intermediary streams while heating the reactors from the helium heat sources rather than using intermediary streams to heat the reactor. The flowsheet for the Kemp model is shown in figure A-3, pg 93.

The Kemp model is explained from right to left. CuCl is cooled from 530 °C to 70 °C while air is heated from 25 °C to 490 °C in heat exchanger E-104. Oxygen leaves the reactor at 530 °C. Both oxygen and air are used to heat $CuO.CuCl_2$ from 370 °C to 430 °C. Oxygen exchanges heat in heat exchanger E-101 with $CuO.CuCl_2$, leaving at 385 °C, and is then used to heat the dry $CuCl_2$ in heat exchanger E-115 to 110 °C. Air is used to heat $CuO.CuCl_2$ from 388 °C to 430 °C in heat exchanger E-103 after it exits from heat exchanger E-104 with the molten CuCl and the heat exchanger at 460 ˚C.

Air is used to cool the warm HCl/water mixture using heat exchanger E-110. The HCl/water mixture is cooled to 40 °C from 370 ˚C air is heated to 225 °C in heat exchanger E-110. The heated air from the cooled CuCl is used to preheat water from 250 °C to the required 400 °C in heat exchanger E-100 while the air is cooled to 399 °C from 459 °C. Air from streams 25 and 28 is mixed to produce a new heated air mix at 289 °C, stream 29. The new air stream is used to preheat atmospheric water at 25 °C and 1 bar pressure to 250 °C and 0.5 bars in heat exchanger E-114, leaving at 70 ˚C.

The HCl/water mixture requires additional low-grade waste heat to increase its temperature to 70 °C as shown in the heat source E-102. A pump is used in the model to obtain the required amount of electrical energy for the energy balance. Additional heat is required to increase the dry $CuCl_2$ from 110 °C to the required 370 °C. This heat cannot be supplied by waste heat and is directly derived from the hot helium through heat source E-106.

3.4 Excess steam model.

The fourth model analyses the need for excess steam in the hydrolysis reactor. The model, developed with excess steam, is shown in figure A-4, pg 94.

Using what has been learned during the development of the Kemp model, the Excess model's development follows a similar path. The reactors are heated by the hot helium and the excess water is treated first. Two inlet streams of water are used. The first, stream 8.2, is heated directly by the oxygen in heat exchanger E-117 from 25 °C to 99 °C, leaving with a vapour fraction of 0.02 with the oxygen cooling from 530 °C to 35 °C. The water stream is heated further in heat exchanger E-100 to 400 ˚C, at a pressure of 0.5 bar by air heated by molten CuCl in heat exchanger E-104. The air is first cooled using heat exchanger E-103 with $CuO.CuCl_2$ to 446 ˚C while heating the $CuO.CuCl_2$ to 430 ˚C.

The excess water is converted to steam by the HCl/water stream leaving the hydrolysis reactor. Excess water enters heat exchanger E-107 after preheating and leaves at 322 °C while the HCl/water mixture enter at 370 °C, exiting at 54 °C.

The preheating section, which can be seen at the top right between MIX-102 and TEE-102, has the excess water split such that as much heat as possible can be extracted from the air or the HCl/water mixture. The heat of the excess air is exchanged in heat exchanger E-102, where the water enters at 25 °C and leaves at 39 °C. The excess HCl/water is cooled from 54 °C to 53 °C in heat exchanger E-111. The pump is used to determine the electrical requirements for the energy balance.

3.5 The variation models

Three additional models are derived from the Kemp model. The models form part of the study to determine the economic benefits of using them for the CuCl cycle.

The first model analyses the need for excess steam in the Kemp model. Extra steam is supplied for and fed directly into the hydrolysis reactor using stream 11.

The second model adjusts the heat input values for Qe-needed. The lower amount of heat removed from the stream requires an additional electricity supply. The amount of electricity generated is balanced by the required amount of waste heat for the cycle. There are no additional streams or utilities in the model when compared to the Kemp model.

The third model analyses the air used to cool the molten CuCl. It is assumed that a pressure drop of 5 kPa occurs in every heat exchanger. The air is circulated and only needs to be recompressed to the inlet pressure. The air streams combine in stream 30 and then heat the water and become stream 31. This stream enters the compressor K-100 where it is compressed to the inlet pressure of 200 kPa.

3.6 The helium heating network

At the bottom of each model an elaborate setup for the helium has been inserted. In figures A-1and A-2 the helium is split in the beginning. What follows is a series of coolers such as E-105, E-108 and E-109. The coolers represent heat provided by the hot helium stream; units can be added depending on whether or not additional heat is required. A second cooler with an energy stream Qth is attached where the stream is split. This energy stream gives a direct indication of how much heat energy from the hot helium is provided and used throughout the cycle.

In figures A-3 and A-4 the stream is split a second time into the heat provided for the reactors and heat supplied for the production of electricity. The split is required to determine whether or not the gas can be split in order to provide conditions that are optimally suitable for the simulation.

3.7 Thermo-physical properties

The thermo-physical data for the individual compounds were found wherever possible in the Unisim^{TM} library. Chemicals that were not present in the library were created artificially. The compounds are CuCl, $CuCl_2$ and $CuO.CuCl_2$. The values shown in table 3-3 were found in Zamfirenscu, Dincer and Naterer (2009) except for the specific heat of CuCl.

Table 3-1: Thermo-physical properties which were not found in the Unisim^{TM} library

Substance	Density (kg/m^3)	Molar mass (kg/kgmole)	Heat of formation (kJ/kgmole)	Specific heat capacity (kJ/kg.K)
CuCl	4220	98.999	$-1.3682x10^5$	0.9*
$CuCl_2$	3400	134.452	$-2.0585X10^5$	0.6
$CuO.CuCl_2$	4080	214	$-3.851x10^5$	0.251

* explained in the next paragraph

CuCl’s heat capacity presents a problem in that it passes through at least two crystalline phase changes. The energy input from 70 °C to 530 °C has been documented by Jaber, Naterer and Dincer (2010) and is shown in figure 3-3.

Jaber, Naterer & Dincer (2010) achieved full heat recovery by exchanging air over molten CuCl after leaving the decomposition reactor. The full amount of heat recovered from 70 °C to 530 °C is condensed into a single Cp value of 0.9 kJ/kg.K. In the simulation, molten CuCl is immediately cooled to 70 °C by air in a heat exchanger. The transition of the crystal phase changes is avoided and the correct amount of heat is obtained for the model by using a single Cp value.

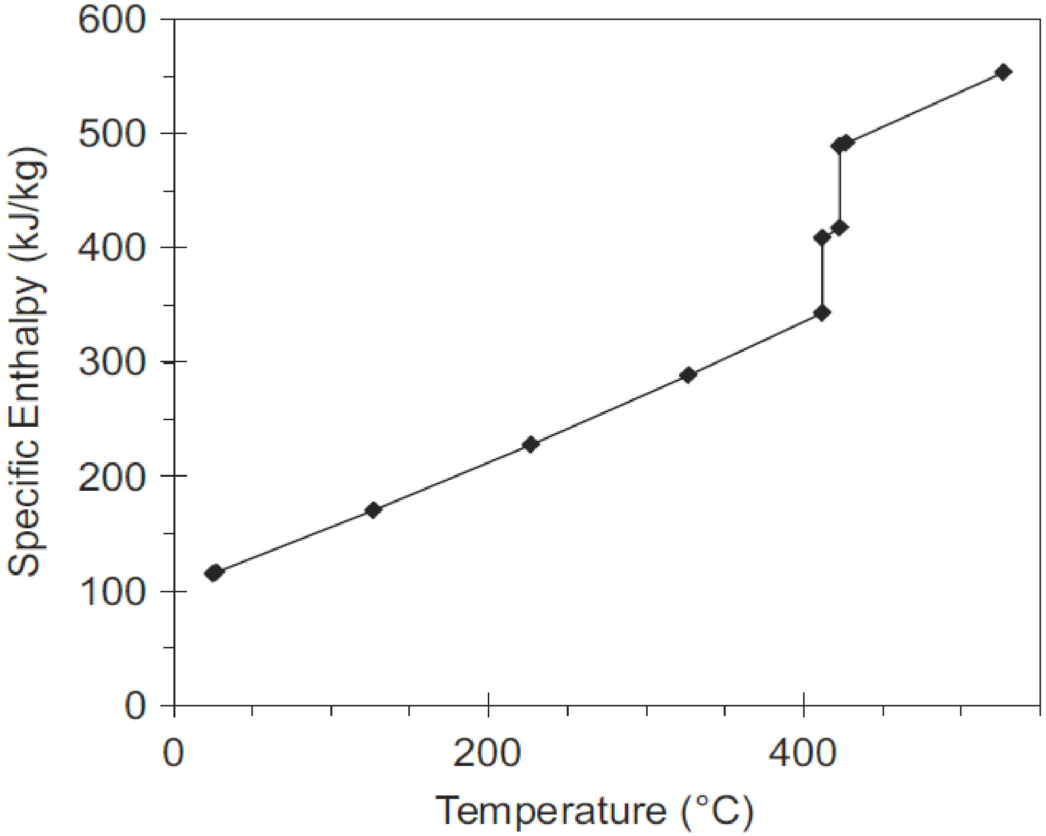

Figure 3-3: CuCl specific enthalpy variation with temperature
(Jaber, Naterer & Dincer, 2010)

3.8 Economics

An economic analysis for the HyS process as proposed by Cilliers (2010: 74) is presented in table 3-2.

Table 3-2: Hydrogen production cost summary according to Cilliers (2010)

	Cilliers Case US$/kg	**Weight %**
Total capital charge	**1.44**	**26**
Overnight capital	1.21	22
Replacement capital	0.22	4
Total fixed O&M	**0.67**	**12**
Annual labour	0.01	0
Insurance	0.11	2
Maint. And repairs	0.55	10
Total variable O&M	**3.67**	**68**
Catalyst, Chemical, filters	0.17	3
Electricity consumed	2.09	38
Nuclear heat	1.35	25
Steam cost	0.00	0
Water consumed	0.07	1
By-product credit	**-0.34**	**-6**
Total hydrogen cost	**5.44**	**100**

For this study it is assumed the capital charge and the total fixed operational and maintenance costs for the CuCl cycle and the HyS process will be the same. The total variable operation and maintenance cost will change as the variables vary between models and the two processes. The final economic analysis is presented with all the models in one table for a more direct comparison in section 4.4.

4. Results and discussion

A description of the CuCl cycle is presented in chapter 3. Four different models of the CuCl cycle are presented which differ only in the way the heat-exchanger network is laid out. The models are labelled the Base model, the Canadian model, the Kemp model and the Excess model. Chapter 4 presents each of these models in the simulation software package Unisim^{TM} where the models are individually analysed. The mass-and-energy balances for each model are presented in a tabulated format in the appendix.

The model's source consisting of helium which flows at 160 kg/s or 576,000 kg/h, enters the cycle at 750 °C, leaves at 300 °C and delivers 350 MW_t of useful thermal energy. The actual temperature of 720.1 °C used in the model serves to obtain 350 MW of thermal energy with a helium exit temperature of 300 °C. The loss in temperature from 750 ˚C to 720.1 ˚C is heat lost to the environment and is not simulated. Helium will be distributed throughout the model. The mass flow rates of the feed streams in all the models are adjusted until all the heat has been used.

An economic analysis will be performed on all the optimised models. This study will not present a fully detailed economic analysis which is considered beyond the scope of this mini-dissertation. The economic analysis provided by Cilliers (2010) is used as a template when determining the cost of Hydrogen production.

To conduct the economic analysis it is assumed, for the purpose of this mini-dissertation, the fixed capital cost, labour cost, maintenance cost, water cost and chemical and catalyst cost will be the same for both the HyS cycle and the CuCl cycle. To obtain the correct values for the costs mentioned above it will have to be multiplied by a factor. The value of this factor is considered beyond the scope of this mini-dissertation. The only change in the economics for this mini-dissertation is the amount of thermal and electrical energy used, the amount of hydrogen produced, and the amount of steam imported.

Results are presented for each model. The mass and mole balance for each stream is presented in section 4-1 and shown in tables 4-1 to 4-4. The mass and mole fractions are presented in the appendices for each model. The energy balances are presented in section 4.2.

The energy balance is based on a model which is used to calculate the amount of electrical energy required to produce 1 kgmole/s hydrogen to be used in the electrolyser. Following this, the amount of electrical energy which will be required by the larger models according to Faraday's law will be calculated using this model. Finally the required amount of electrical energy is converted to an equivalent amount of thermal energy. This amount will be substituted into the model to determine the flow rates of the material streams and to complete the energy balance.

All the models will receive electrical energy from the helium heat source. It is assumed that, all of the electricity required by all the models, except one, is produced from the helium.

A number of energy streams are labelled "QNA". These streams contribute to Unisim^{TM} and the values presented by energy streams in the model are neither accurate, nor useful nor necessary. These energy streams are used to persuade Unisim^{TM} that a stream is liquid in order to obtain an accurate value from the pump for the electrolyser. The electrolyser's energy is calculated in the model shown in section 4.2.

Three additional models will be presented next. The models do not form part of the main evaluation but are rather used to identify external additions which can be made to improve the cycle or possibly to become a factor at a later stage during final development of the cycle.

The economic analysis is based on work performed by Cilliers (2010) on the HyS process. At the time of this study very little information was available on the potential economics of the 4-step cycle, although various studies have been done on the corresponding 5-step cycle. The results obtained from the economic analysis will be compared directly to that of the HyS cycle.

Tables and figures labelled A-X are shown in the appendix.

4.1 Mass Balance

Base case

The Base case shown in Unisim^{TM} is set out in figure A-1, pg 91. Table 4-1 shows the mass balance for the Base case where hydrogen is produced at a basis of 160 kg/s helium which delivers 350 MW of thermal energy.

Table 4-1: Essential-streams mass balance for Base case

Name	Molar flow (kgmole/h)	Mass flow (kg/h)
1- HCl	6,870	208,245
2- CuCl	4,580	453,415
3- H_2	2,340	5,513.25
5- $CuCl_2$ dry	4,580	615,794
8- H_2O Cold	4,580	82,509.2
10 - $CuOCuCl_2$	2,290	490,057
12- Oxygen	1,145	36,640
16- HCl + H_2O	6,870	208,245
20- He in	143,900	576,000

The mass fraction of hydrogen in stream 3 is 0.84. The Base case represents only the amount of heat which will be required for the heating of the reactors. The heating and cooling of certain streams within the cycle will have a value assigned but heating will come from an imaginary heat or cooling source. The minimum amount of heat required in the cycle is presented in this case. Thus 4,616.24 kg/h of hydrogen is produced for the Base case when 350 MW_t of heat is used.

The value given in table 4-1 for the hydrogen flow is different from that presented in the text whereas the former presents the amount of material flowing within the stream which also contains water; the value in the text is the amount of hydrogen actually produced. The complete mass and mole fractions of each component are given in table A-1, pg 98.

Canadian model

The Canadian model was developed by interpreting figure 3-1. The model uses the energy which is released by the molten CuCl when it is cooled to 70 ˚C to heat the hydrolysis reactor. An interpretation of figure 3-1 for Unisim^{TM} is shown in figure A-2, pg 92. The mass balances for essential streams are shown in table 4-2. The complete mass-and-energy balance is shown in table A-2, pg 104.

Table 4-2: Mass balance of the Canadian model.

Name	**Molar flow (kgmole/h)**	**Mass flow (kg/h)**
1- HCl	6,084	184,420
2- CuCl	4,056	401,540
3- H_2	2,057	4,608.63
4- $CuCl_2$	6,055	581,355
9- H_2O cold	4,056	73,069.2
13- $CuOCuCl_2$	2,028	433,989
15- Oxygen	1,014	32,448
19- HCl + H_2O	6,084	184,420
24- Air	1.17E+04	336,367
31- He in	1.44E+05	576,000

At a helium flow of 160 kg/s, the Canadian model delivers 4,088 kg/h hydrogen with a thermal efficiency of 38.95 % LHV.

An interpretation of the Canadian model with excess steam, presented by Ferrandon *et al.* (sa) in figure 3-2, was built unsuccessfully in Unisim^{TM}. The mass-and-energy balances of the model do not match the values obtained in Unisim^{TM}. For example, the amount of heat required for the cycle to heat the water did not match the value for the Canadian model, and the amount of heat released by the molten CuCl did not match the values used in Unisim^{TM}. These differences make it impossible to build a replica model that answers to specifications; hence no evaluation can be performed on this model.

Kemp model

The Kemp model differs from the Canadian model in the method employed to use the heat from the molten CuCl. The Kemp model uses molten CuCl mainly to heat the water indirectly, first it heats air which is then transferred around the system, whereas in the Canadian model the CuCl is used to heat the hydrolysis reactor directly. The mass balance for selected streams in the Kemp model as shown in figure A-3, pg 93, is shown in table 4-3 and the complete mass balance is given in table A-3, pg 110.

Table 4-3: Mass balance for the Kemp model.

Name	**Molar Flow (kgmole/h)**	**Mass Flow (kg/h)**
1- HCl	6,390	193,695
2- CuCl	4,260	421,736
3-H_2	2,160	4,840.42
4- $CuCl_2$	6,360	610,595
8- Water	4,260	76,744.3
11- $CuOCuCl_2$	2,130	455,817
14- Oxygen	1,065	34,080
19- HCl + H_2O	6,390	193,695
24- Air	2.13E+04	612,702
26- Air	1.23E+04	353,285
40- He In	1.44E+05	576,000

With a flow of 160 kg/s of helium as basis, hydrogen is produced at a rate of 4,294 kg/h. The thermal efficiency of this model is 40.89 % LHV.

Excess model

The Excess model differs from the Kemp and Canadian models in that it uses a more realistic amount of water for the hydrolysis reactor. The addition of water requires more high-quality energy. If helium is used to provide high quality heat lower efficiency can be expected as less heat can then be used to produce hydrogen. The water must be heated using recycled heat in the model. The model layout is shown in figure A-4, pg 94, the mass balance in table 4-4, and the complete mass balance in table A-4 pg 117.

Table 4-4: Mass balance for the Excess model.

Name	**Molar Flow (kgmole/h)**	**Mass Flow (kg/h)**
1- HCl	6,096	184,783
2- CuCl	4,064	402,332
3- H_2	2,061	4,617.72
4- $CuCl_2$	6,067	582,502
8.2 (Water in)	2,337	42,097.7
11- $CuOCuCl_2$	2,032	434,845
13- Oxygen	1,016	32,512
17 - Air	1.17E+04	337,031
22 - HCl + H_2O	2.67E+04	556,341
26 - Extra water	2.24E+04	402,674
40 - Helium	1.44E+05	576,000

With a helium flow of 160 kg/s as basis, hydrogen is produced at 4,096 kg/h. The thermal efficiency of the cycle is 39.01 % LHV.

Three additional models are discussed in a later section. These models entail a compressor for the air, steam which is bought, and electricity which is bought.

4.2 Energy balance

Electrolyser

The energy needed by the electrolyser is required to complete an energy balance for the CuCl cycle. The portion of electrical energy required for the model is directly related to the amount of hydrogen produced. A model has been developed from the work done by Cilliers (2010) and is used to calculate the electrical energy required for various amounts of hydrogen produced.

The theory of the model is explained in section 2.4. Table 4-5 displays this model for a basis of 1 kgmole/s hydrogen. The cell potential is 0.65 V.

Table 4-5: Electrolyser calculation for 1 kgmole/s hydrogen

H_2 Produced	**1**	**kgmole/s**
Cell potential	0.65	V
$2CuCl + 2Cl^- \rightarrow 2CuCl_2 + 2e^-$		
$2H^+ + 2e^- \rightarrow H_2$		
For 1 kgmole/s		
1 Ampere	1	C/s
$1e^-$	$1.6020E^{-19}$	C
1 kgmole of electrons	$6.0220E^{+26}$	electrons
# Electrons per reaction	2	
	=	
Electrolyser current	192,944,880	C/s
Multiply by Voltage	0.65	V
	=	
Electrolyser power (P = I.V)	**125,414,172**	**W**

The above model is designed so that the amount of hydrogen produced can be changed and the amount of electrical energy required can be calculated.

The total electrical requirements of any model depends not only on what is needed for the electrolyser, but also on what the pump needs that transfers the aqueous hydrochloric acid after it exits the hydrolyser. In one of the extra Kemp models a compressor is used to move air used to cool molten CuCl. The electricity required for this operation will be generated from the helium. A more in-depth discussion on the compressor is done at a later stage.

The electricity is generated from the helium. It is assumed that the energy conversion from heat to electricity is 40 %. The equivalent amount of thermal energy required for the electrolyser can be calculated from this value.

The energy balances are shown in the next few pages. The amount of electrical energy required to produce 1 kgmole/s is 125,414,172 W. The total electrical energy requirement for the electrolyser is obtained by multiplying this total by the number of kgmole per second of hydrogen produced in the model. The amount of electrical energy required from pumps and compressors is added to obtain the total amount of electrical energy converted to an equivalent thermal amount. This value is placed in the model as Qe-needed. The energy balances for heaters and cooler are shown next. QNA and its derivatives are not shown as they do not form part of the energy balance.

Base case

The electrolyser calculations for the Base case are shown in table 4-6 below and the energy balance is shown in table 4-7.

Table 4-6: Electrolyser calculation for the Base case.

	Base case	
Hydrogen production	2,290	kgmole/h
Conversion to kgmole/s	0.6361	kgmole/s
Electrolyser electrical energy requirement for 1 kgmole/s hydrogen	125,414,172	W
Electrolyser electrical power requirement for 0.6361 kgmole/s hydrogen	**79,777,348.3**	**W**
	79.78	MW
Q Pump	0.15	MW
Total Electrical energy required	**79.93**	**MW**
Thermal Energy requirement	**199.82**	**MW**

The total electrical energy requirement is supplied from the helium.

Table 4-7: Energy balance and utilities for the Base case.

Name	**Heat Flow (MW)**
Q $CuCl_2$ heat	29.56
Q Pump	0.15
Q supercool	63.10
Q-$CuOCuCl_2$	5.10
Q-O_2	5.07
QCuCl	51.01
Qe-needed	**199.82**
QHCl	18.12
QR2	49.31
QR3	100.56
Qth	349.70
Qwater	73.30

Canadian

The electrolyser calculations for the Canadian case are shown in table 4-8 and the energy balance is shown in table 4-9.

Table 4-8: Electrolyser calculations for the Canadian Model

	Canadian case	
Hydrogen production	2,028	kgmole/h
Conversion to kgmole/s	0.5633	kgmole/s
Electrolyser electrical energy requirement for 1 kgmole/s hydrogen	125,414,172	W
Electrolyser electrical power requirement for 0.5633 kgmole/s hydrogen	**70,649,983.56**	**W**
	70.65	MW
Q pump	0.13	MW
Total Electrical energy required	**70.78**	**MW**
Thermal Energy requirement	**176.96**	**MW**

Table 4-9: Energy balance for the Canadian model.

Name	**Heat Flow (MW)**
Q air	10.26
Q extra H_2O	45.97
Q pump	0.13
Q-$CuOCuCl_2$	4.51
Qe-needed	**176.96**
QR2	43.67
QR3	89.06
Qth	349.91

Kemp

The electrolyser calculations for the Kemp model are shown in table 4-10 below and the energy balance is shown in table 4-11.

Table 4-10: Electrolyser calculation for the Kemp model.

	Kemp model	
Hydrogen production	2,130	kgmole/h
Conversion to kgmole/s	0.5917	kgmole/s
Electrolyser electrical energy requirement for 1 kgmole/s hydrogen	125,414,172	W
Electrolyser electrical power requirement for 0.5917 kgmole/s hydrogen	**74,203,385.10**	**W**
	74.20	MW
Q pump	0.14	MW
Total Electrical energy required	**74.34**	**MW**
Thermal Energy requirement	**185.86**	**MW**

Table 4-11: Energy balance for the Kemp model.

Name	**Heat Flow (MW)**
Q $CuCl_2$ heat	24.76
Q pump	0.14
Q waste extra	18.43
Qe-needed	**185.86**
QR2	45.87
QR3	93.54
Qth	350.02

Excess

The Excess energy balance is shown in table 4-8

Table 4-12: Electrolyser calculation for the Excess model

	Excess model	
Hydrogen production	2,032	kgmole/h
Conversion to kgmole/s	0.5644	kgmole/s
Electrolyser electrical energy requirement for 1 kgmole/s hydrogen	125,414,172	W
Electrolyser electrical power requirement for 0.5644 kgmole/s hydrogen	**70,789,332.64**	**W**
	70.79	MW
Q pump	0.43	MW
Total Electrical energy required	**71.22**	**MW**
Thermal Energy requirement	**178.05**	**MW**

Table 4-13: Energy balance for the Excess model.

Name	**Heat Flow (MW)**
Q $CuCl_2$ heat	26.23
Q extra heat	19.05
Q pump	0.43
Qe-needed	**178.05**
QR2	37.45
QR3	89.23
Qth	350.01

The helium is split twice in both the Kemp model and the Excess model. The first involves stream 40 and 51 in both models. Stream 51 goes to a cooler where Qth is determined. Qth is the heat delivered by the hot helium which comes from the high-temperature nuclear reactor. This value is as close to 350 MW as possible. The top stream is split again as it supplies helium to heat the reactors while the bottom stream is used to convert the heat to electrical energy.

Table 4-14: Split stream temperatures

	Kemp		**Excess**	
Split (R-E)	**Stream from Reactor (°C)**	**Stream from electricity (°C)**	**Stream from reactor (°C)**	**Stream from electricity (°C)**
50-50	326	279	307	292
60 - 40	391	162	376	185

The split can be changed from 50-50 to 60-40 without any change in the outlet temperature of 300 ˚C. Meanwhile only the individual streams' temperature changes as shown in table 4-14. It can be concluded here that the streams can be split to best advantage for the reactors and the electricity generated.

4.3 Results for variation models

The Kemp model is of the available range the best and delivers hydrogen at the lowest price. The option of buying electricity to increase output or to buy steam to maintain the model is explored in the next section. Included as well is the issue of the air which is used as a cooling medium and to meet transport requirements. These options are analysed in discussing.

Kemp model with extra steam

The Kemp model is stoichiometrically correct, but the lack of excess steam for the hydrolyser is unrealistic. The following model explores the possibility of buying excess steam for the Kemp model then compares the model with the Excess model to determine whether or not the purchasing of steam should be investigated further. It is assumed that steam is bought at $25/ton and delivered at 400 ˚C.

The layout of the model is shown in figure A-5, pg 95. The mass balance is shown in table 4-15 with the complete mass-and-energy balance shown in table A-5, pg 125. The electrolyser requirements are shown in table 4-16 and the energy balance is shown in table 4-17.

Table 4-15: Mass balance of the Kemp model with extra steam.

Name	**Molar Flow (kgmole/h)**	**Mass Flow (kg/h)**
1- HCl	6,500	197,030
2- CuCl	4,333	428,991
3- H_2	2,197	4,924.04
4- $CuCl_2$	6,469	621,101
8 Water	13,000	234,196
11 - Steam bought	13,000	234,196
12- $CuOCuCl_2$	2,167	463,659
15- Oxygen	1,083	34,666.60
20- HCl + H2O	28,170	587,356
24- Air	121,300	3,490,240
26- Air	12,490	359,363
40- He In	143,900	576,000

Table 4-16: Electrolyser requirement for the Kemp model with steam

	Kemp model	
Hydrogen production	2,166.67	kgmole/h
Conversion to kgmole/s	0.6019	kgmole/s
Electrolyser electrical power requirements for 1 kgmole/s hydrogen	125,414,172	W
Electrolyser electrical power requirements for 0.6019 kgmole/s hydrogen	**75,480,751.67**	**W**
	75.48	MW
Q pump	0.40	MW
Total electrical energy required	**75.88**	**MW**
Thermal energy requirement	**189.71**	**kW**

Table 4-17: Energy balance of the Kemp model with extra steam.

Name	**Heat Flow (MW)**
Q $CuCl_2$ heat	25.18
Q pump	0.40
Qe-needed	**189.71**
QR2	39.93
QR3	95.15
Qth	349.98

Kemp Model with bought electricity

Electricity can be bought from an outside source at \$75/MW$_e$.h which matches the conversion efficiency of electricity generated from thermal sources at 40 %. Waste heat is used within the drying process and to heat a process stream.

The model is shown in figure A-6, pg 96.The mass balance of essential streams are shown in table 4-18 and the complete mass balance is shown in table A-6, pg 131. The amount of waste heat which is required and the electricity generated from the helium are shown in table 4-19. The electrolyser requirement and the amount of electricity which needs to be bought are shown in table 4-20 and the energy balance is shown in table 4-21. The waste heat generated as the loss of heat from the high-temperature reactor is not included and is assumed to be lost to the environment.

Table 4-18: Mass balance for Kemp model where electricity is bought.

Name	**Molar flow (kgmole/h)**	**Mass flow (kg/h)**
1- HCl	7,095	215,065
2- CuCl	4,730	468,265
3- H_2	2,399	5,374.46
4- $CuCl_2$	7,062	677,961
8- Extra water	4,730	85,211.4
11- $CuOCuCl_2$	2,365	506,107
14- Oxygen	1,183	37,840
19- HCl + H2O	7,095	215,065
24- Air	23,650	680,301
26- Air	13,640	392,263
40- He In	143,900	576,000

Table 4-19: Waste heat requirement for the Kemp model.

Waste Heat		
# moles of H_2 produced	2,365	kgmole/h
Conversion to kmole/s	0.6569	kgmole/s
Qdryer requirement	122	MJ/kgmole
Q requirement for dryer	80.15	MW
Qwaste for heating extra stream	20.47	MW
Total waste heat required	**100.61**	**MW**
Minimum Heat for electricity	**167.69**	**MW**
Electricity generated	**67.08**	**MW**

Table 4-20: Electrical requirement for Kemp model.

	Kemp Model	
Hydrogen production	2365	kgmole/h
Conversion to kgmole/s	0.8128	kgmole/s
Electrolyser electrical power requirements for 1 kgmole/s hydrogen	125,414,172	W
Electrolyser electrical power requirements for 0.8128 kmole/s hydrogen	**101,936,639**	**W**
P = I.V	101.94	MW
Q pump	0.13	MW
Total electrical energy required	**102.07**	**MW**
Electrical energy generated	**67.08**	**MW**
Electricity bought	**34.99**	**MW**

Table 4-21: Energy balance for the Kemp model with electricity bought.

Name	**Heat Flow (MW)**
Q $CuCl_2$ heat	27.49
Q pump	0.16
Qe-needed	**167.69**
QR2	50.93
QR3	103.86
Qth	349.96
Qwaste	20.47

Kemp model with a compressor

Air is used as a cooling medium for molten CuCl. All of the previous models, except for where it is required, it is assumed a zero pressure drop. This model explores a pressure drop of 5 kPa within the heat exchangers for the air and the need to re-compress the air.

The compressor's electrical energy is generated from the helium stream. The model explores further what the economic factors would be. Figure A-7, pg 97, gives the layout of the model, Table 4-22 give the mass balance of the model, table A-7, pg 138, gives the complete mass and energy balances, table 4-23 gives the electrical input and table 4-24 gives the energy balance for the model.

Table 4-22: Mass balance of Kemp model with a compressor.

Name	Molar Flow (kgmole/h)	Mass Flow (kg/h)
1- HCl	6,210	188,239
2- CuCl	4,140	409,856
3- H_2	2,099	4,704.07
4- $CuCl_2$	6,181	593,395
8 Water	4,140	74,582.50
11- $CuOCuCl_2$	2,070	442,977
14- Oxygen	1,035	33,120
19- HCl + H2O	6,210	188,239
24- Air	20,700	595,443
26- Air	11,940	343,334
31- Air	32,640	938,777
40- He In	143,900	576,000

Table 4-23: Electrical requirement for the Kemp model with a compressor.

	Kemp model	
Hydrogen production	2070	kgmole/h
Conversion to kgmole/s	0.5750	kgmole/s
Electrolyser electrical power requirements for 1 kgmole/s hydrogen	125,414,172	W
Electrolyser electrical power requirements for 0.5750 kgmole/s hydrogen	**72,113,148.90**	**W**
	72.11	MW
Q Pump	0.14	MW
Q comp	3.68	MW
Total electrical energy required	**75.94**	**MW**
Thermal energy requirement	**189.84**	**kW**

Table 4-24: Energy balance for Kemp model with compressor.

Name	**Heat flow (MW)**
Q comp	3.68
Q $CuCl_2$ heat	24.06
Q pump	0.14
Q waste extra	17.91
Qe-needed	**189.84**
QR2	44.57
QR3	90.90
Qth	349.37

4.4 Economics

The economics are based on the work performed by Cilliers (2010:74) as reported in section 3.7 above. The only variables which differ are the amount of energy and the number of moles of hydrogen formed. For the present study the cost of delivery of various products is shown in table 4-24.

Table 4-25: Cost of delivery for energy and external sources.

Thermal	30	US$/MWth.h
Electrical	75	US$/MWe.h
Steam	25	US$/ton steam
Oxygen	40	US$/ton O_2

The economic analysis of every model is shown in table 4-25 for a direct comparison. The best model of Cilliers (2010) is also compared. It is assumed that the cost of water is the same amount for both the HyS process and the CuCl cycle.

Table 4-26: Combined economic analysis of all the models

	US$/kg H_2							
	Cilliers Case	**Base**	**Canadian**	**Kemp**	**Excess**	**Kemp - Steam**	**Kemp - Electricity**	**Kemp - Compressor**
Total capital charge	**1.44**	**1.44**	**1.44**	**1.44**	**1.44**	**1.44**	**1.44**	**1.44**
Overnight capital	1.21	1.21	1.21	1.21	1.21	1.21	1.21	1.21
Replacement capital	0.22	0.22	0.22	0.22	0.22	0.22	0.22	0.22
Total fixed O&M	**0.67**	**0.67**	**0.67**	**0.67**	**0.67**	**0.67**	**0.67**	**0.67**
Annual labour	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
Insurance	0.11	0.11	0.11	0.11	0.11	0.11	0.11	0.11
Maint. and repairs	0.55	0.55	0.55	0.55	0.55	0.55	0.55	0.55
Total variable O&M	**3.67**	**2.51**	**2.81**	**2.69**	**2.80**	**3.98**	**2.69**	**2.75**
Catalyst, Chemical, filters	0.17	0.17	0.17	0.17	0.17	0.17	0.17	0.17
Electricity consumed	2.09	0.00	0.00	0.00	0.00	0.00	**0.24**	0.00
Nuclear heat	1.35	2.27	2.57	2.45	2.56	**2.40**	**2.20**	**2.51**
Steam cost	0.00	0.00	0.00	0.00	0.00	**1.34**	0.00	0.00
Water consumed	0.07	0.07	0.07	0.07	0.07	0.07	0.07	0.07
By-product credit	**-0.34**	**-0.32**	**-0.32**	**-0.32**	**-0.32**	**-0.32**	**-0.32**	**-0.32**
Total Hydrogen cost	**5.44**	**4.31**	**4.60**	**4.48**	**4.60**	**5.78**	**4.48**	**4.54**

4.4 Discussion

This mini-dissertation on the CuCl model evaluates whether or not the cycle is better suited as a potential hydrogen production method than the HyS process.

The Base case model shows that a thermal efficiency of 44 % is achieved at a cost of US$4.31 /kg for a stoichiometric model with heat supplied only to the reactors and an assumption that all the heat required is imaginary. This value is the upper efficiency limit and the lower limit in the potential cost of the CuCl cycle, if the full 350 MW_t of heat is used by the reactors. The potential thermal efficiency of the Base case is 13.3 % higher than the 30.7 % which was obtained by Cilliers (2010) for the HyS process.

The University of Ontario Institute of Technology in Canada is currently doing the bulk of research on the CuCl cycle and in the process has developed a number of models shown in figures 3-1 and figure 3-2. Figure 3-1 is a simulated stoichiometric model that attained to a thermal efficiency of 38.95 % and produces hydrogen at US$4.60/kg.

The CuCl cycle consists of three chemical reactions and a drying step. The excess steam required for the hydrolysis reaction in the cycle is not simulated in the stoichiometric models hence a new model has to be used. The model for excess steam developed in Canada is shown in figure 3-2. Attempts were made to simulate this model in the simulation software Unisim^{TM} used in this mini-dissertation, but the attempts were unsuccessful. The difference in the steam calculation is attributed a difference in the thermo-physical properties of the various chemicals, a difference in the mass flow rates used, and a difference between the simulation packages, which therefore requires each model to be constructed differently.

The CuCl cycle cannot be evaluated with exclusive reference to this model. A new model which uses a different heat-exchange network needs to be developed in Unisim^{TM} to evaluate the CuCl cycle.

The stoichiometric Kemp model achieved a thermal efficiency of 40.89 % and delivers hydrogen at a cost of US$4.48/kg. It also offers a positive difference in thermal efficiency of 1.88 % compared to the Canadian stoichiometric model, achieves an improved of 10.19 % in thermal efficiency and is cheaper by US$0.96/kg H_2 when compared to the HyS process.

As with the Canadian model, the Kemp model needs to take account of the need for excess steam. The Excess model is a derivative of the Kemp model with changes to the water-preheat stream. A different method of preheating the water is required. The model's thermal efficiency is down to 39.01 % and hydrogen is produced at US$4.60/kg H_2, but this cycle includes provision for the need for excess steam. The drop in efficiency is due to the need to use high-quality heat to assist heating part of the water stream and not to heat the reactors and thereby decrease the amount of hydrogen which can be produced.

The Kemp model is the best of all the models discussed above, but this assessment is made on certain assumptions. Three models were built to test these assumptions by determining the effect of the external add-ons.

It is assumed that all the electricity required for the electrolyser stream is generated by the helium stream. The Kemp model is adjusted to determine the amount of waste energy required and the amount of electricity generated in the production of the waste heat. The remaining electricity requirement will be bought. The thermal efficiency of the cycle is 45.41 %. The cost of hydrogen remains the same as that of the Kemp model where no electricity is bought. The thermal efficiency does not reflect the bought electricity.

The Kemp model is a stoichiometric model without excess steam. Steam is bought at US$20/ton and it is assumed the steam is at 400 °C. It is supplied directly to the hydrolysis reactor. The amount of steam added to the system is equal to the amount of feed-water used for the cycle as it gives the best overall conversion for the cycle. The thermal efficiency of the cycle is 41.6 %, but the additional cost of buying steam increases the cost of the hydrogen to US$5.78/kg, which is US$0.34/kg more expensive than the HyS process and US$1.18/kg more expensive than the excess model. It is therefore not recommended to buy steam for this cycle.

Air is used to cool the molten CuCl from 530 °C to 70 °C and it enters at 200 kPa. It is assumed throughout the cycle that there is no drop in pressure for the air stream as it passes through a heat exchanger. The Kemp model was tested by adding a 5 kPa pressure drop over every heat exchanger for the air. It was further assumed that the air flows in a closed circuit and only needs to be compressed from 180 kPa to 200 kPa as it leaves the last heat exchanger. The Kemp model where the air is recompressed has a thermal efficiency of 39.81 % and produces hydrogen at a cost of US$4.54/kg, which is only a US$0.06/kg increase in cost. Thus the need for a compressor only devalues the product by 1.48 %.

The results obtained from the study reported in this mini-dissertation clearly show that the CuCl cycle is potentially less expensive and less energy intensive than the HyS process. The reduction of cost due to materials of construction, the lesser need for a catalyst and the lower operating temperature will further reduce the cost requirement. Additional costs will be incurred for labour due to the involvement of solids operating in the cycle.

Hydrogen is produced at a lower cost and a higher efficiency than the HyS process thus the CuCl can be considered to be a more viable cycle than the HyS process for the production of hydrogen in combination with a nuclear source such as an HTR.

5. Conclusion and Recommendations

5.1 Conclusion

The copper-chloride cycle was evaluated in this mini-dissertation to determine whether it is a suitable option to enlist in the production of hydrogen from a nuclear source and to compare it with the hybrid sulphur (HyS) cycle.

The evaluation started with the development of four models in Unisim^{TM}. The Base model only shows heat requirements for the reactors and the heat flows of individual streams. The Canadian model is developed in Canada for the CuCl cycle. The model is presented both stoichiometrically and with the need for excess steam. The approach exemplified in the Kemp model (third model) developed by the author is different from that applied in developing the Canadian model. The Kemp model was also adjusted to serve the need for excess steam in a non-stoichiometric case. The CuCl cycle has been compared to the HyS cycle by using the study of Cilliers (2010) as a basis for comparison of performance and economic analysis.

The Base model is unrealistic due to the lack of an energy source and an incomplete energy balance which means it cannot be used for the purpose of direct comparison. It does however provide a basis from which other models can be built and decisions can be made on how a heat exchange network can be developed.

Canadian researchers have developed two models. The stoichiometric model is more energy intensive than the Kemp model due to a need to heat water for the hydrolysis reactor. The author was unable to develop the non-stoichiometric Canadian model with excess steam in Unisim^{TM} which is similar to the model developed by Ferrandon *et al.* (sa).

The Kemp model provided the best efficiency and cost of all the models. The efficiency of the model is 40.89 % which is 10.19 % better than the HyS model. The model also produces hydrogen at a cost of US$4.48/kg which is US$0.96/kg less than the HyS costs. When a more realistic model like the Excess model is compared, hydrogen can be produced at US$4.6/kg which is US$0.84/kg cheaper. The thermal efficiency of this model is 39 % which is an improved efficiency of 8.6 % compared to the HyS cycle.

It can be concluded in comparison with the HyS process that the CuCl cycle is more advantageous, both in cost and thermal efficiency which merits further investigation

Additional models were developed to determine whether or not the cycle can be improved. The additional factors included purchasing electricity and steam and the need to use a compressor. It is recommended that steam must not be purchased as it increased the cost by US$1.30/kg to US$5.78/kg, making the cycle more expensive than the HyS process. If a compressor is used to circulate air to cool molten CuCl in a closed-loop system, the cost will be increased by US$0.06/kg. The addition of a compressor will only increase the cost by 1.49 %. Electricity prices change during the day due to peak demand and would vary the production cost. Factoring in the buying of electricity at US$75/$MW_e$ for the purpose of this mini-dissertation neither decreased nor increased the cost. As electricity prices vary during the day a form of load-following can be implemented to increase daily production.

5.2 Recommendations

The evaluation done for the purpose of this mini-dissertation has proven that the CuCl cycle merits further investigation. The Kemp model shows potential, but its feed-stream values are based in theory and not in practice. A number of assumptions were made. The following is a list of recommendations for future work to be performed on the CuCl cycle.

- The electrolyser needs to be studied in more detail to provide a better model to calculate the electrical energy requirements for future work.
- The hydrolysis reactor's requirement for excess steam needs to be investigated further. An investigation needs to be performed on the reactor to lower the amount of steam required for the reactor.
- As the price of electricity varies due to peak demand during the day, it can be purchased at a lower price. The purchased electricity can be used to produce hydrogen at a lower price and in greater quantities. The disadvantage of using this technique is that most utilities do not like to vary production flow. The advantages of this technique are evident and must be investigated further to determine its implementation potential.
- The use of air in the cycle has proven that it can operate efficiently. Better materials which can perform the task of air need to be investigated as higher heat flow rates will require that less heat be wasted once the stream has used all its useful heat.
- With respect to water removed in the dryer as steam mixed with air, an investigation is required into recycling the water back into the cycle.
- A new cycle which was discovered by Wang *et al.* (2009) has the potential to lower the energy requirements and place less strain on the construction materials. This cycle requires further investigation and compare to the CuCl cycle treated in this minidissertation.
- The author was unable to produce the model presented by Ferrandon *et al*. (sa) with Unisim^{TM}. This model is not amendable to discussion of its suitability or correctness. It needs to be constructed and evaluated in Aspen^{TM} for a more complete evaluation on the CuCl cycle.
- The splitting of the helium stream has the potential to offer two streams with different operating temperatures. An investigation needs to be performed to

determine whether the best operating conditions can be secured by splitting the hot helium stream.

- Carbon nanotubes have been shown to double the amount of hydrogen produced when it is used for water electrolysis (Dubey *et al.*, 2010). Replacing the electrodes with carbon nanotubes can increase the production of hydrogen and needs to be investigated further.
- The expected capital and operational cost of the HyS cycle differ to that of the CuCl cycle. This mini-dissertation assumed the costs are the same. More studies have to be done to obtain more accurate cost figures of the CuCl cycle to more accurately compare the two cycles.

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APPENDIX

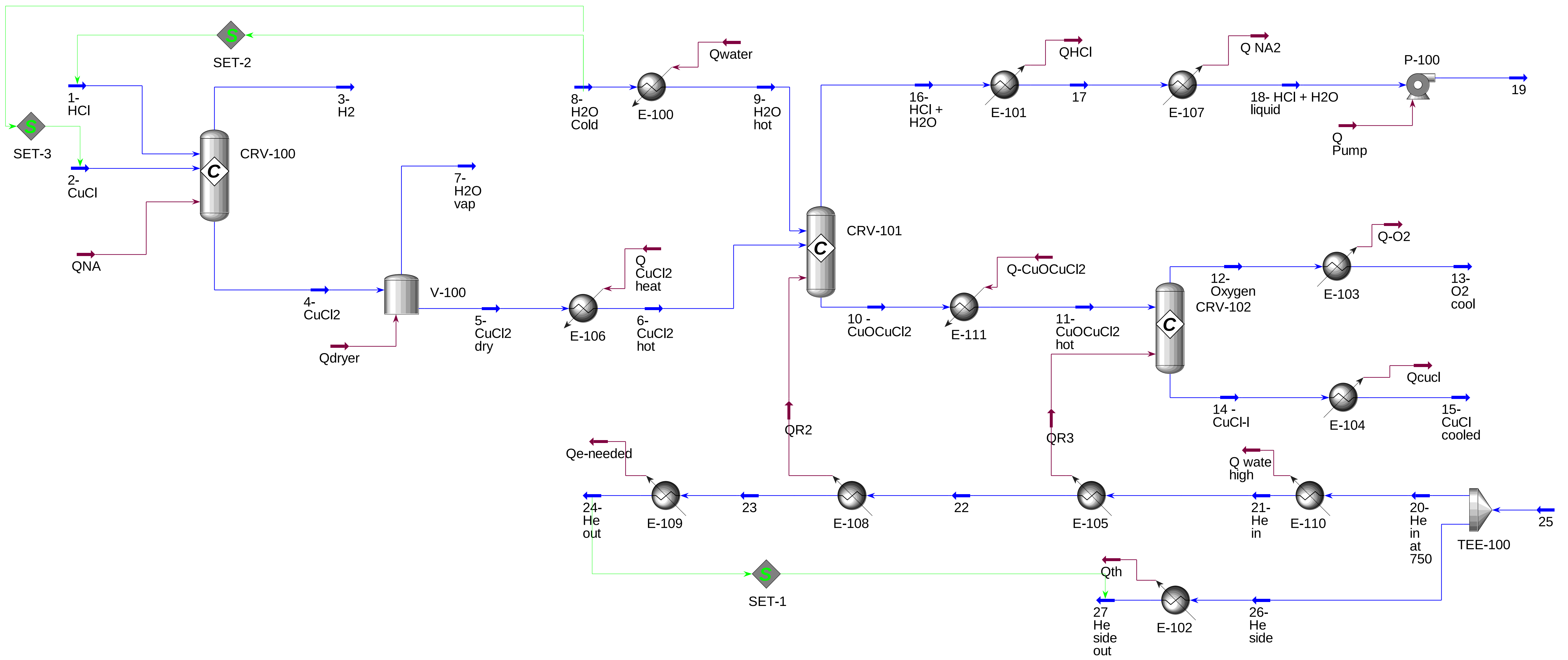


Figure A-1: Layout of Base Model

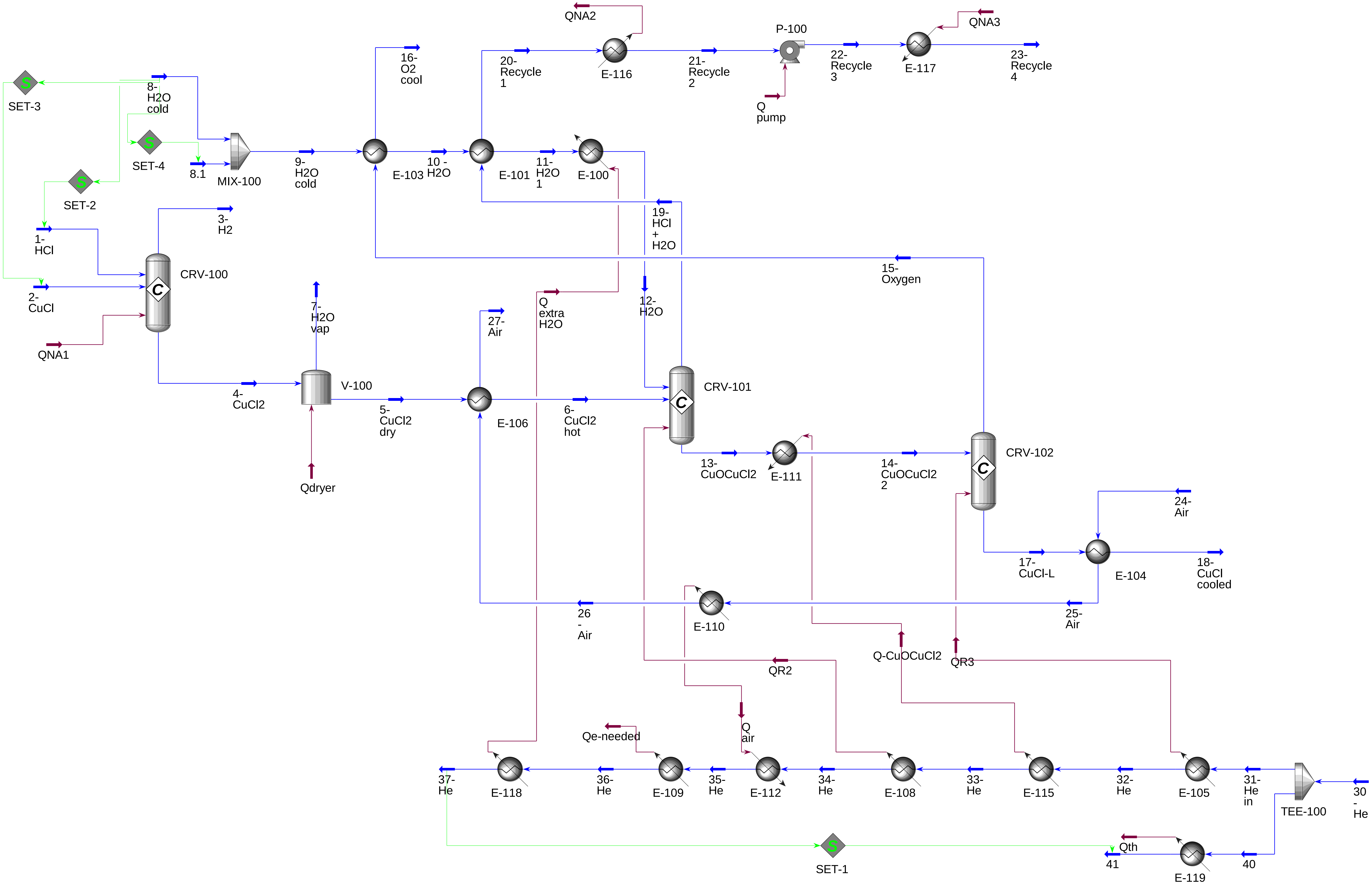


Figure A-2: Layout of Canadian Model

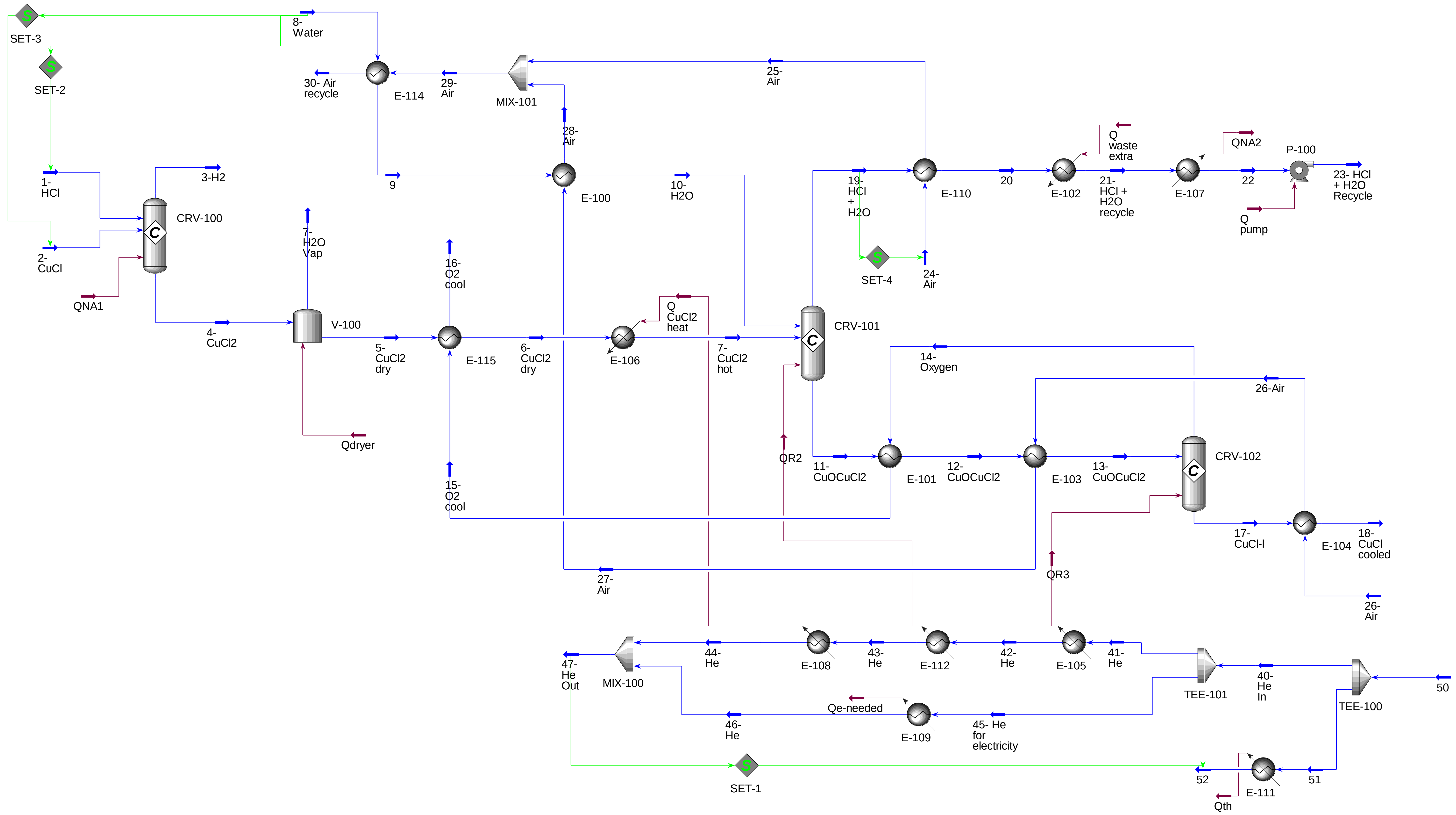


Figure A-3: Layout of Kemp Model

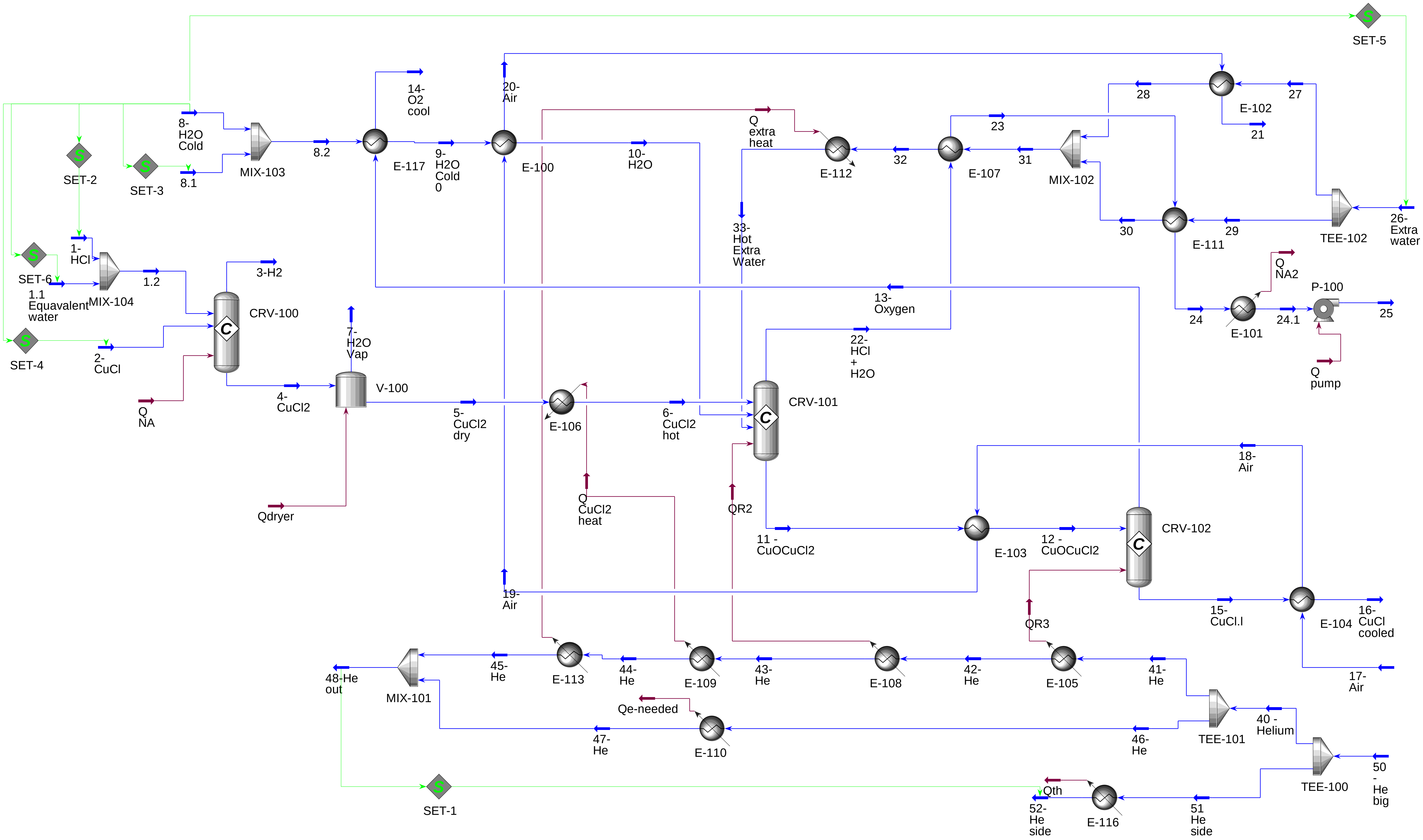


Figure A-4: Layout of Excess Model

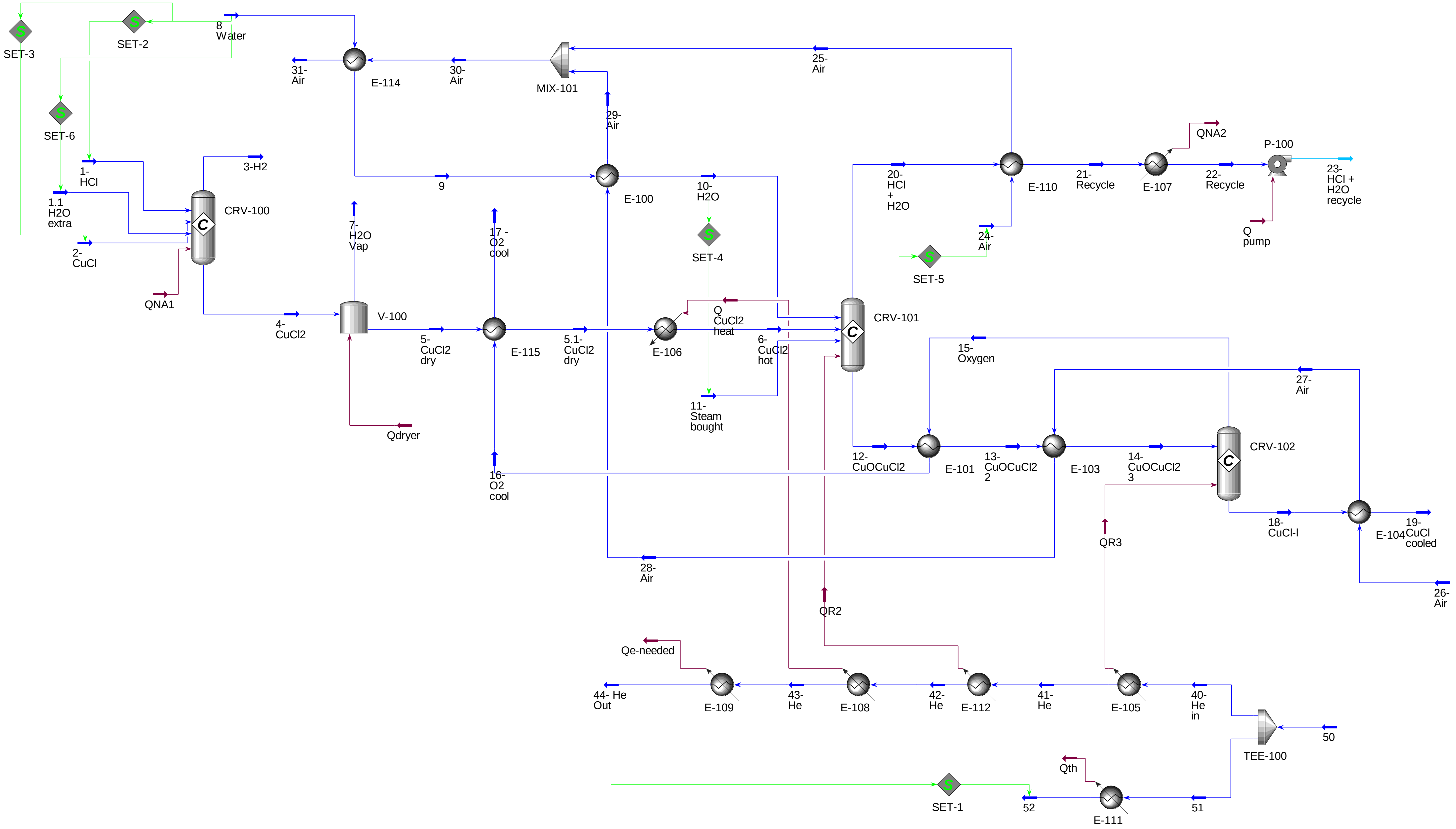


Figure A-5: Layout of Kemp Model with extra steam

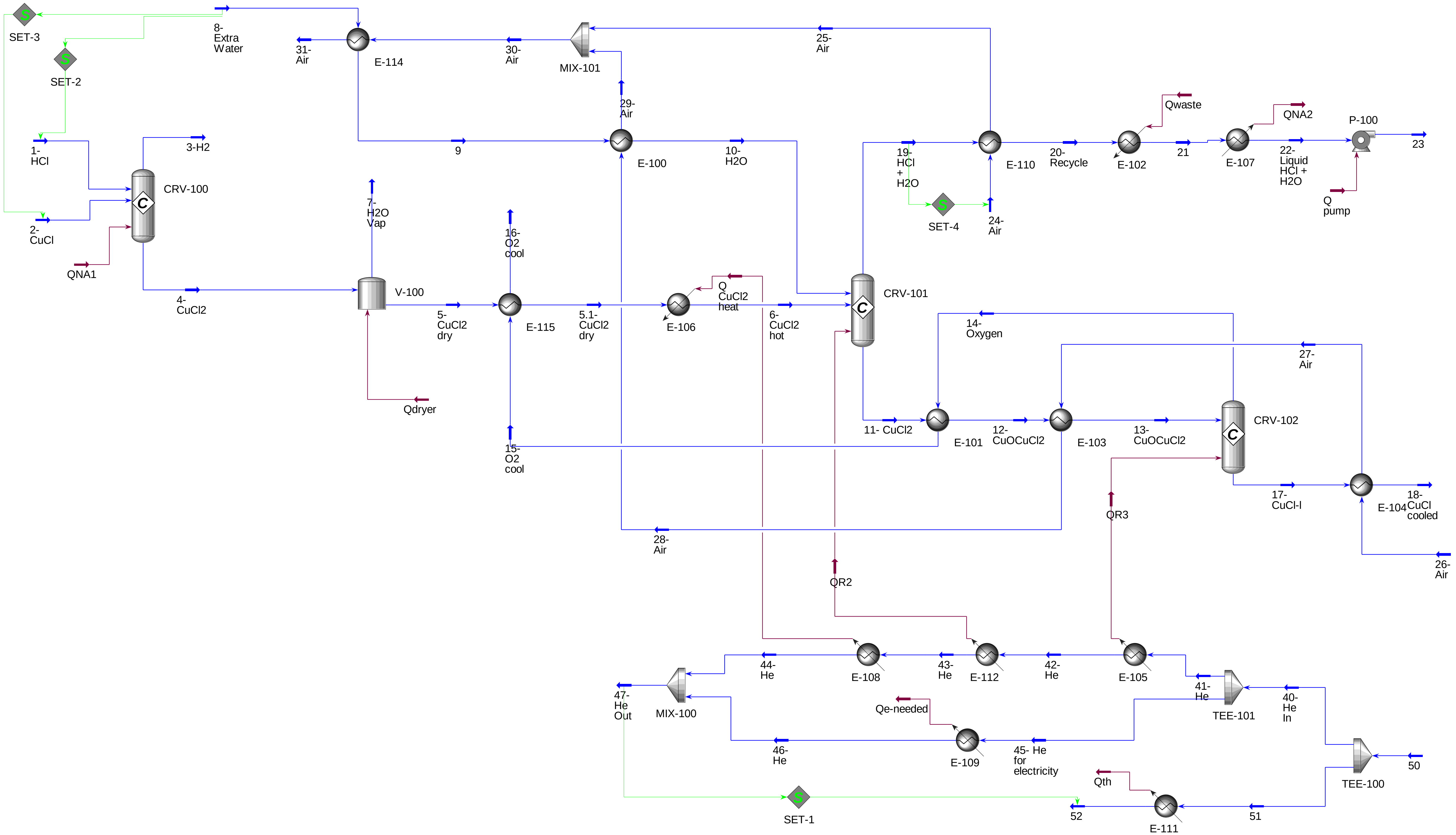


Figure A-6: Layout of Kemp Model where electricity is purchased

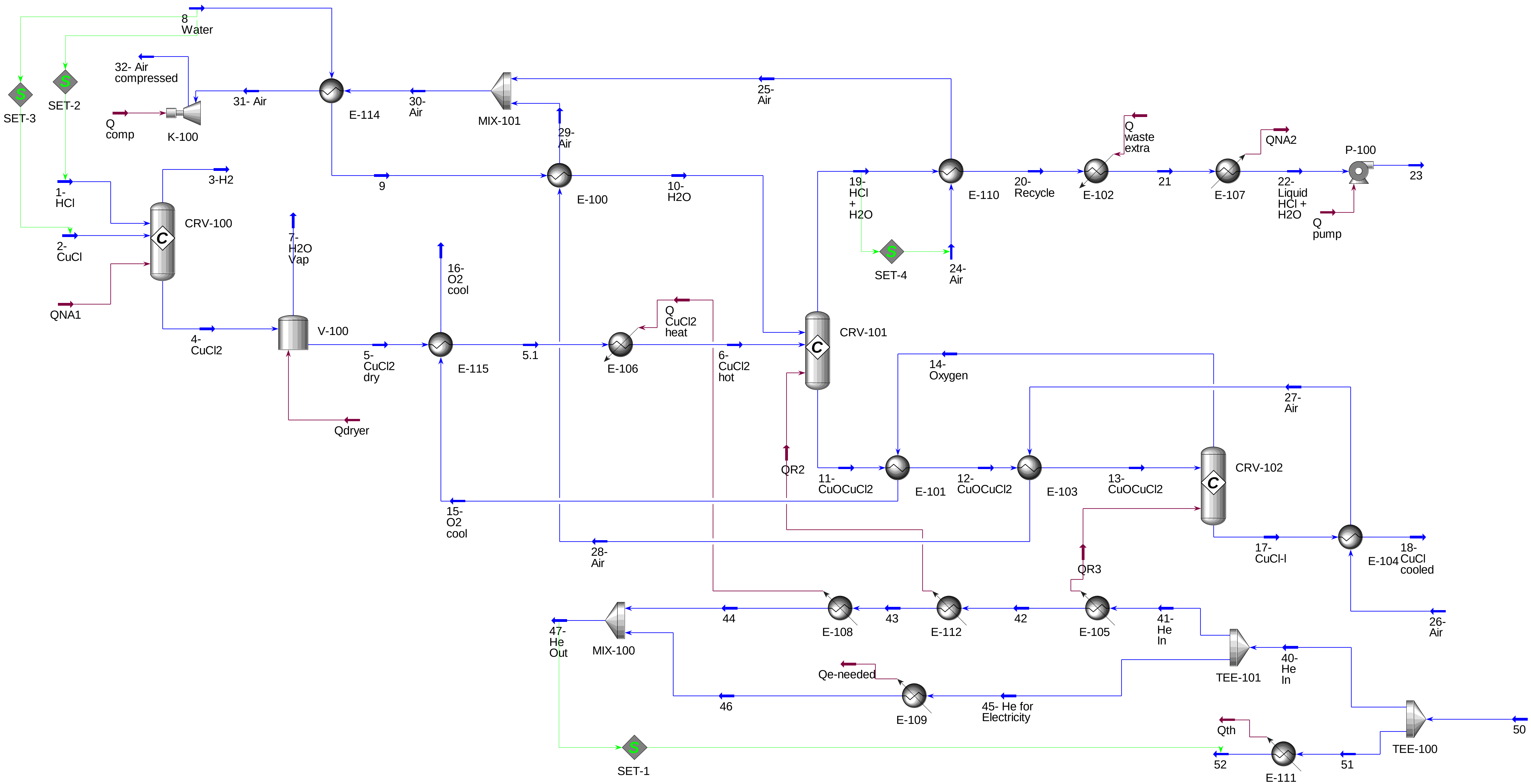


Figure A-7: Layout of Kemp Model with a compressor

Table A-1: Mass and Energy Balance for the Base Model

Streams

Fluid Pkg: All

Name	1- HCl	2- CuCl	3- H2	4- CuCl2	5- CuCl2 dry
Vapour Fraction	0.6812	0.0000	1.0000	0.0000	0.0000
Temperature (C)	80.00 *	80.00 *	80.00	80.00 *	82.00
Pressure (kPa)	2400 *	2400 *	2400	2400	50.00 *
Molar Flow (kgmole/h)	6870.0	4580.0	2339.6	6820.5	4580.0
Mass Flow (kg/h)	208245	453415	5513.25	656152	615794
Std Ideal Liq Vol Flow (m3/h)	233.2	109.5	66.98	221.6	181.1
Heat Flow (MW)	-294.472326	-167.825893	-2.32598814	-431.660897	-256.038293
Molar Enthalpy (kJ/kgmole)	-1.543e+005	-1.319e+005	-3579	-2.278e+005	-2.013e+005
Comp Mass Frac (CuCl*)	0.0000 *	1.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (HCl)	0.8019 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (Helium)	0.0000 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (CuO.CuCl2*)	0.0000 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (CuCl2*)	0.0000 *	0.0000 *	0.0000	0.9385	1.0000
Comp Mass Frac (H2O)	0.1981 *	0.0000 *	0.1627	0.0615	0.0000
Comp Mass Frac (Hydrogen)	0.0000 *	0.0000 *	0.8373	0.0000	0.0000
Comp Mass Frac (Oxygen)	0.0000 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl*)	0.0000 *	1.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (HCl)	0.6667 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (Helium)	0.0000 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (CuO.CuCl2*)	0.0000 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl2*)	0.0000 *	0.0000 *	0.0000	0.6715	1.0000
Comp Mole Frac (H2O)	0.3333 *	0.0000 *	0.0213	0.3285	0.0000
Comp Mole Frac (Hydrogen)	0.0000 *	0.0000 *	0.9787	0.0000	0.0000
Comp Mole Frac (Oxygen)	0.0000 *	0.0000 *	0.0000	0.0000	0.0000

Name	6- CuCl2 hot	7- H2O vap	8- H2O Cold	9- H2O hot	10 - CuOCuCl2
Vapour Fraction	0.0000	1.0000	0.0000	1.0000	0.0000
Temperature (C)	370.0 *	82.00 *	25.00 *	400.0 *	370.0 *
Pressure (kPa)	50.00	50.00 *	101.3 *	50.00 *	50.00
Molar Flow (kgmole/h)	4580.0	2240.4	4580.0 *	4580.0	2290.0
Mass Flow (kg/h)	615794	40358.0	82509.2	82509.2	490057
Std Ideal Liq Vol Flow (m3/h)	181.1	40.45	82.68	82.68	120.1
Heat Flow (MW)	-226.480102	-149.301482	-364.136292	-290.831604	-217.409493
Molar Enthalpy (kJ/kgmole)	-1.780e+005	-2.399e+005	-2.862e+005	-2.286e+005	-3.418e+005
Comp Mass Frac (CuCl*)	0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (HCl)	0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (Helium)	0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (CuO.CuCl2*)	0.0000	0.0000	0.0000	0.0000 *	1.0000
Comp Mass Frac (CuCl2*)	1.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (H2O)	0.0000	1.0000	1.0000	1.0000 *	0.0000
Comp Mass Frac (Hydrogen)	0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (Oxygen)	0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (CuCl*)	0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (HCl)	0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (Helium)	0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (CuO.CuCl2*)	0.0000	0.0000	0.0000	0.0000 *	1.0000
Comp Mole Frac (CuCl2*)	1.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (H2O)	0.0000	0.9999	1.0000	1.0000 *	0.0000
Comp Mole Frac (Hydrogen)	0.0000	0.0001	0.0000	0.0000 *	0.0000
Comp Mole Frac (Oxygen)	0.0000	0.0000	0.0000	0.0000 *	0.0000

Streams (continued)

Fluid Pkg: All

Name	11- CuOCuCl2 hot	12- Oxygen	13- O2 cool	14 - CuCl-l	15- CuCl cooled
Vapour Fraction	0.0000	1.0000	1.0000	0.0000	0.0000
Temperature (C)	430.0 *	530.0 *	25.00 *	530.0	80.00 *
Pressure (kPa)	101.3 *	101.3	101.3	101.3	2400 *
Molar Flow (kgmole/h)	2290.0	1145.0	1145.0	4580.0	4580.0
Mass Flow (kg/h)	490057	36640.0	36640.0	453419	453419
Std Ideal Liq Vol Flow (m3/h)	120.1	32.21	32.21	109.5	109.5
Heat Flow (MW)	-212.313910	5.06654577	-3.03511173e-003	-116.817603	-167.827250
Molar Enthalpy (kJ/kgmole)	-3.338e+005	1.593e+004	-9.543	-9.182e+004	-1.319e+005
Comp Mass Frac (CuCl*)	0.0000	0.0000	0.0000	1.0000	1.0000
Comp Mass Frac (HCl)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Helium)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuO.CuCl2*)	1.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuCl2*)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (H2O)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Hydrogen)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Oxygen)	0.0000	1.0000	1.0000	0.0000	0.0000
Comp Mole Frac (CuCl*)	0.0000	0.0000	0.0000	1.0000	1.0000
Comp Mole Frac (HCl)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Helium)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuO.CuCl2*)	1.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl2*)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (H2O)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Hydrogen)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Oxygen)	0.0000	1.0000	1.0000	0.0000	0.0000

Name	16- HCl + H2O	17	18- HCl + H2O liquid	19	20- He in at 750
Vapour Fraction	1.0000	1.0000	0.0000 *	0.0000	1.0000
Temperature (C)	370.0	70.00 *	-95.85	-95.37	750.0 *
Pressure (kPa)	50.00	50.00	50.00	2400 *	3000
Molar Flow (kgmole/h)	6870.0	6870.0	6870.0	6870.0	1.4389e+005
Mass Flow (kg/h)	208245	208245	208245	208245	576000
Std Ideal Liq Vol Flow (m3/h)	233.2	233.2	233.2	233.2	4643
Heat Flow (MW)	-250.590942	-268.710047	-331.814914	-331.662920	602.922613
Molar Enthalpy (kJ/kgmole)	-1.313e+005	-1.408e+005	-1.739e+005	-1.738e+005	1.508e+004
Comp Mass Frac (CuCl*)	0.0000	0.0000	0.0000	0.0000	-0.0000
Comp Mass Frac (HCl)	0.8019	0.8019	0.8019	0.8019	-0.0000
Comp Mass Frac (Helium)	0.0000	0.0000	0.0000	0.0000	1.0000
Comp Mass Frac (CuO.CuCl2*)	0.0000	0.0000	0.0000	0.0000	-0.0000
Comp Mass Frac (CuCl2*)	0.0000	0.0000	0.0000	0.0000	-0.0000
Comp Mass Frac (H2O)	0.1981	0.1981	0.1981	0.1981	-0.0000
Comp Mass Frac (Hydrogen)	0.0000	0.0000	0.0000	0.0000	-0.0000
Comp Mass Frac (Oxygen)	0.0000	0.0000	0.0000	0.0000	-0.0000
Comp Mole Frac (CuCl*)	0.0000	0.0000	0.0000	0.0000	-0.0000
Comp Mole Frac (HCl)	0.6667	0.6667	0.6667	0.6667	-0.0000
Comp Mole Frac (Helium)	0.0000	0.0000	0.0000	0.0000	1.0000
Comp Mole Frac (CuO.CuCl2*)	0.0000	0.0000	0.0000	0.0000	-0.0000
Comp Mole Frac (CuCl2*)	0.0000	0.0000	0.0000	0.0000	-0.0000
Comp Mole Frac (H2O)	0.3333	0.3333	0.3333	0.3333	-0.0000
Comp Mole Frac (Hydrogen)	0.0000	0.0000	0.0000	0.0000	-0.0000
Comp Mole Frac (Oxygen)	0.0000	0.0000	0.0000	0.0000	-0.0000

Streams (continued)

Fluid Pkg: All

Name		21- He in	22	23	24- He out	25
Vapour Fraction		1.0000	1.0000	1.0000	1.0000	1.0000
Temperature	(C)	720.8 *	599.9	540.6	300.4	750.0
Pressure	(kPa)	3000 *	3000	3000	3000	3000
Molar Flow	(kgmole/h)	1.4389e+005	1.4389e+005	1.4389e+005	1.4389e+005	2.8779e+005
Mass Flow	(kg/h)	576000	576000	576000	576000 *	1.15200e+006
Std Ideal Liq Vol Flow	(m3/h)	4643	4643	4643	4643	9286
Heat Flow	(MW)	578.639862	478.077009	428.765737	228.942383	1205.84523
Molar Enthalpy	(kJ/kgmole)	1.448e+004	1.196e+004	1.073e+004	5728	1.508e+004
Comp Mass Frac (CuCl*)		0.0000 *	0.0000	0.0000	0.0000	-0.0000
Comp Mass Frac (HCl)		0.0000 *	0.0000	0.0000	0.0000	-0.0000
Comp Mass Frac (Helium)		1.0000 *	1.0000	1.0000	1.0000	1.0000
Comp Mass Frac (CuO.CuCl2*)		0.0000 *	0.0000	0.0000	0.0000	-0.0000
Comp Mass Frac (CuCl2*)		0.0000 *	0.0000	0.0000	0.0000	-0.0000
Comp Mass Frac (H2O)		0.0000 *	0.0000	0.0000	0.0000	-0.0000
Comp Mass Frac (Hydrogen)		0.0000 *	0.0000	0.0000	0.0000	-0.0000
Comp Mass Frac (Oxygen)		0.0000 *	0.0000	0.0000	0.0000	-0.0000
Comp Mole Frac (CuCl*)		0.0000 *	0.0000	0.0000	0.0000	-0.0000
Comp Mole Frac (HCl)		0.0000 *	0.0000	0.0000	0.0000	-0.0000
Comp Mole Frac (Helium)		1.0000 *	1.0000	1.0000	1.0000	1.0000
Comp Mole Frac (CuO.CuCl2*)		0.0000 *	0.0000	0.0000	0.0000	-0.0000
Comp Mole Frac (CuCl2*)		0.0000 *	0.0000	0.0000	0.0000	-0.0000
Comp Mole Frac (H2O)		0.0000 *	0.0000	0.0000	0.0000	-0.0000
Comp Mole Frac (Hydrogen)		0.0000 *	0.0000	0.0000	0.0000	-0.0000
Comp Mole Frac (Oxygen)		0.0000 *	0.0000	0.0000	0.0000	-0.0000

Name		26- He side	27 He side out	Q CuCl2 heat	Q NA2	Q Pump
Vapour Fraction		1.0000	1.0000	---	---	---
Temperature	(C)	750.0	300.4	---	---	---
Pressure	(kPa)	3000	3000	---	---	---
Molar Flow	(kgmole/h)	1.4389e+005	1.4389e+005	---	---	---
Mass Flow	(kg/h)	576000	576000	---	---	---
Std Ideal Liq Vol Flow	(m3/h)	4643	4643	---	---	---
Heat Flow	(MW)	602.922613	228.942383	29.5581906	63.1048672	0.151993309
Molar Enthalpy	(kJ/kgmole)	1.508e+004	5728	---	---	---
Comp Mass Frac (CuCl*)		-0.0000	-0.0000	---	---	---
Comp Mass Frac (HCl)		-0.0000	-0.0000	---	---	---
Comp Mass Frac (Helium)		1.0000	1.0000	---	---	---
Comp Mass Frac (CuO.CuCl2*)		-0.0000	-0.0000	---	---	---
Comp Mass Frac (CuCl2*)		-0.0000	-0.0000	---	---	---
Comp Mass Frac (H2O)		-0.0000	-0.0000	---	---	---
Comp Mass Frac (Hydrogen)		-0.0000	-0.0000	---	---	---
Comp Mass Frac (Oxygen)		-0.0000	-0.0000	---	---	---
Comp Mole Frac (CuCl*)		-0.0000	-0.0000	---	---	---
Comp Mole Frac (HCl)		-0.0000	-0.0000	---	---	---
Comp Mole Frac (Helium)		1.0000	1.0000	---	---	---
Comp Mole Frac (CuO.CuCl2*)		-0.0000	-0.0000	---	---	---
Comp Mole Frac (CuCl2*)		-0.0000	-0.0000	---	---	---
Comp Mole Frac (H2O)		-0.0000	-0.0000	---	---	---
Comp Mole Frac (Hydrogen)		-0.0000	-0.0000	---	---	---
Comp Mole Frac (Oxygen)		-0.0000	-0.0000	---	---	---

* Specified by user.

Streams (continued)

Fluid Pkg: All

Name	Q wate high	Q-CuOCuCl2	Q-O2	Qcucl	Qdryer
Vapour Fraction	---	---	---	---	---
Temperature (C)	---	---	---	---	---
Pressure (kPa)	---	---	---	---	---
Molar Flow (kgmole/h)	---	---	---	---	---
Mass Flow (kg/h)	---	---	---	---	---
Std Ideal Liq Vol Flow (m3/h)	---	---	---	---	---
Heat Flow (MW)	24.2827517	5.09558294	5.06958088	51.0096473	26.3211218
Molar Enthalpy (kJ/kgmole)	---	---	---	---	---
Comp Mass Frac (CuCl*)	---	---	---	---	---
Comp Mass Frac (HCl)	---	---	---	---	---
Comp Mass Frac (Helium)	---	---	---	---	---
Comp Mass Frac (CuO.CuCl2*)	---	---	---	---	---
Comp Mass Frac (CuCl2*)	---	---	---	---	---
Comp Mass Frac (H2O)	---	---	---	---	---
Comp Mass Frac (Hydrogen)	---	---	---	---	---
Comp Mass Frac (Oxygen)	---	---	---	---	---
Comp Mole Frac (CuCl*)	---	---	---	---	---
Comp Mole Frac (HCl)	---	---	---	---	---
Comp Mole Frac (Helium)	---	---	---	---	---
Comp Mole Frac (CuO.CuCl2*)	---	---	---	---	---
Comp Mole Frac (CuCl2*)	---	---	---	---	---
Comp Mole Frac (H2O)	---	---	---	---	---
Comp Mole Frac (Hydrogen)	---	---	---	---	---
Comp Mole Frac (Oxygen)	---	---	---	---	---

Name	Qe-needed	QHCl	QNA	QR2	QR3
Vapour Fraction	---	---	---	---	---
Temperature (C)	---	---	---	---	---
Pressure (kPa)	---	---	---	---	---
Molar Flow (kgmole/h)	---	---	---	---	---
Mass Flow (kg/h)	---	---	---	---	---
Std Ideal Liq Vol Flow (m3/h)	---	---	---	---	---
Heat Flow (MW)	199.823354 *	18.1191046	28.3113300	49.3112719	100.562853
Molar Enthalpy (kJ/kgmole)	---	---	---	---	---
Comp Mass Frac (CuCl*)	---	---	---	---	---
Comp Mass Frac (HCl)	---	---	---	---	---
Comp Mass Frac (Helium)	---	---	---	---	---
Comp Mass Frac (CuO.CuCl2*)	---	---	---	---	---
Comp Mass Frac (CuCl2*)	---	---	---	---	---
Comp Mass Frac (H2O)	---	---	---	---	---
Comp Mass Frac (Hydrogen)	---	---	---	---	---
Comp Mass Frac (Oxygen)	---	---	---	---	---
Comp Mole Frac (CuCl*)	---	---	---	---	---
Comp Mole Frac (HCl)	---	---	---	---	---
Comp Mole Frac (Helium)	---	---	---	---	---
Comp Mole Frac (CuO.CuCl2*)	---	---	---	---	---
Comp Mole Frac (CuCl2*)	---	---	---	---	---
Comp Mole Frac (H2O)	---	---	---	---	---
Comp Mole Frac (Hydrogen)	---	---	---	---	---
Comp Mole Frac (Oxygen)	---	---	---	---	---

* Specified by user.

Streams (continued)

Fluid Pkg: All

Name		Qth	Qwater			
Vapour Fraction		---	---			
Temperature	(C)	---	---			
Pressure	(kPa)	---	---			
Molar Flow	(kgmole/h)	---	---			
Mass Flow	(kg/h)	---	---			
Std Ideal Liq Vol Flow	(m3/h)	---	---			
Heat Flow	(MW)	373.980230	73.3046876			
Molar Enthalpy	(kJ/kgmole)	---	---			
Comp Mass Frac (CuCl*)		---	---			
Comp Mass Frac (HCl)		---	---			
Comp Mass Frac (Helium)		---	---			
Comp Mass Frac (CuO.CuCl2*)		---	---			
Comp Mass Frac (CuCl2*)		---	---			
Comp Mass Frac (H2O)		---	---			
Comp Mass Frac (Hydrogen)		---	---			
Comp Mass Frac (Oxygen)		---	---			
Comp Mole Frac (CuCl*)		---	---			
Comp Mole Frac (HCl)		---	---			
Comp Mole Frac (Helium)		---	---			
Comp Mole Frac (CuO.CuCl2*)		---	---			
Comp Mole Frac (CuCl2*)		---	---			
Comp Mole Frac (H2O)		---	---			
Comp Mole Frac (Hydrogen)		---	---			
Comp Mole Frac (Oxygen)		---	---			

Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc Level
CRV-101	Conversion Reactor	9- H2O hot 6- CuCl2 hot QR2	10 - CuOCuCl2 16- HCl + H2O QR2	No	500.0 *
CRV-102	Conversion Reactor	11- CuOCuCl2 hot QR3	14 - CuCl-l 12- Oxygen QR3	No	500.0 *
CRV-100	Conversion Reactor	1- HCl 2- CuCl QNA	4- CuCl2 3- H2 QNA	No	500.0 *
E-103	Cooler	12- Oxygen	13- O2 cool Q-O2	No	500.0 *
E-104	Cooler	14 - CuCl-l	15- CuCl cooled Qcucl	No	500.0 *
E-101	Cooler	16- HCl + H2O	17 QHCl	No	500.0 *
E-105	Cooler	21- He in	22 QR3	No	500.0 *
E-108	Cooler	22	23 QR2	No	500.0 *
E-109	Cooler	23	24- He out Qe-needed	No	500.0 *
E-102	Cooler	26- He side	27 He side out Qth	No	500.0 *
E-107	Cooler	17	18- HCl + H2O liquid Q NA2	No	500.0 *
E-110	Cooler	20- He in at 750	21- He in Q wate high	No	500.0 *
E-111	Heater	10 - CuOCuCl2 Q-CuOCuCl2	11- CuOCuCl2 hot	No	500.0 *
E-100	Heater	8- H2O Cold	9- H2O hot	No	500.0 *

Unit Ops (continued)

Operation Name	Operation Type	Feeds	Products	Ignored	Calc Level
E-100	Heater	Qwater		No	500.0 *
E-106	Heater	5- CuCl2 dry	6- CuCl2 hot	No	500.0 *
		Q CuCl2 heat			
V-100	Tank	4- CuCl2	5- CuCl2 dry	No	500.0 *
		Qdryer	7- H2O vap		
			Qdryer		
SET-1	Set			No	500.0 *
SET-3	Set			No	500.0 *
SET-2	Set			No	500.0 *
P-100	Pump	18- HCl + H2O liquid	19	No	500.0 *
		Q Pump			
TEE-100	Tee	25	20- He in at 750	No	500.0 *
			26- He side		

Table A-2: Mass and Energy Balance for the Canadian Model

Streams

Fluid Pkg: All

Name		1- HCl	2- CuCl	3- H2	4- CuCl2	5- CuCl2 dry
Vapour Fraction		0.6756	0.0000	1.0000	0.0000	0.0000
Temperature	(C)	70.00 *	70.00 *	70.00	70.00 *	82.00
Pressure	(kPa)	2400 *	2400 *	2400	2400	50.00 *
Molar Flow	(kgmole/h)	6084.0	4056.0	2056.7	6055.3	4056.0
Mass Flow	(kg/h)	184420	401540	4608.63	581355	545341
Std Ideal Liq Vol Flow	(m3/h)	206.5	96.99	59.04	196.5	160.4
Heat Flow	(MW)	-261.980315	-149.628702	-1.20836925	-384.808823	-226.744829
Molar Enthalpy	(kJ/kgmole)	-1.550e+005	-1.328e+005	-2115	-2.288e+005	-2.013e+005
Comp Mass Frac (CuCl*)		0.0000 *	1.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (HCl)		0.8019 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (Helium)		0.0000 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (CuO.CuCl2*)		0.0000 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (CuCl2*)		0.0000 *	0.0000 *	0.0000	0.9380	1.0000
Comp Mass Frac (H2O)		0.1981 *	0.0000 *	0.1129	0.0619	0.0000
Comp Mass Frac (Hydrogen)		0.0000 *	0.0000 *	0.8871	0.0000	0.0000
Comp Mass Frac (Oxygen)		0.0000 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (Nitrogen)		0.0000 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl*)		0.0000 *	1.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (HCl)		0.6667 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (Helium)		0.0000 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (CuO.CuCl2*)		0.0000 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl2*)		0.0000 *	0.0000 *	0.0000	0.6698	1.0000
Comp Mole Frac (H2O)		0.3333 *	0.0000 *	0.0140	0.3301	0.0000
Comp Mole Frac (Hydrogen)		0.0000 *	0.0000 *	0.9860	0.0000	0.0000
Comp Mole Frac (Oxygen)		0.0000 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (Nitrogen)		0.0000 *	0.0000 *	0.0000	0.0000	0.0000

Name		6- CuCl2 hot	7- H2O vap	8- H2O cold	8.1	9- H2O cold
Vapour Fraction		0.0000	1.0000	0.0000	0.0000	0.0000
Temperature	(C)	370.0 *	82.00 *	25.00 *	25.00 *	25.00
Pressure	(kPa)	50.00	50.00 *	101.3 *	101.3 *	101.3
Molar Flow	(kgmole/h)	4056.0	1999.3	2028.0 *	2028.0	4056.0
Mass Flow	(kg/h)	545341	36014.4	36534.6	36534.6	73069.2
Std Ideal Liq Vol Flow	(m3/h)	160.4	36.09	36.61	36.61	73.22
Heat Flow	(MW)	-200.568405	-133.233218	-161.237642	-161.237642	-322.475284
Molar Enthalpy	(kJ/kgmole)	-1.780e+005	-2.399e+005	-2.862e+005	-2.862e+005	-2.862e+005
Comp Mass Frac (CuCl*)		0.0000	0.0000	0.0000 *	0.0000 *	0.0000
Comp Mass Frac (HCl)		0.0000	0.0000	0.0000 *	0.0000 *	0.0000
Comp Mass Frac (Helium)		0.0000	0.0000	0.0000 *	0.0000 *	0.0000
Comp Mass Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000 *	0.0000 *	0.0000
Comp Mass Frac (CuCl2*)		1.0000	0.0000	0.0000 *	0.0000 *	0.0000
Comp Mass Frac (H2O)		0.0000	1.0000	1.0000 *	1.0000 *	1.0000
Comp Mass Frac (Hydrogen)		0.0000	0.0000	0.0000 *	0.0000 *	0.0000
Comp Mass Frac (Oxygen)		0.0000	0.0000	0.0000 *	0.0000 *	0.0000
Comp Mass Frac (Nitrogen)		0.0000	0.0000	0.0000 *	0.0000 *	0.0000
Comp Mole Frac (CuCl*)		0.0000	0.0000	0.0000 *	0.0000 *	0.0000
Comp Mole Frac (HCl)		0.0000	0.0000	0.0000 *	0.0000 *	0.0000
Comp Mole Frac (Helium)		0.0000	0.0000	0.0000 *	0.0000 *	0.0000
Comp Mole Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000 *	0.0000 *	0.0000
Comp Mole Frac (CuCl2*)		1.0000	0.0000	0.0000 *	0.0000 *	0.0000
Comp Mole Frac (H2O)		0.0000	0.9999	1.0000 *	1.0000 *	1.0000
Comp Mole Frac (Hydrogen)		0.0000	0.0001	0.0000 *	0.0000 *	0.0000
Comp Mole Frac (Oxygen)		0.0000	0.0000	0.0000 *	0.0000 *	0.0000
Comp Mole Frac (Nitrogen)		0.0000	0.0000	0.0000 *	0.0000 *	0.0000

* Specified by user.

Streams (continued)

Fluid Pkg: All

Name		10 - H2O	11- H2O 1	12- H2O	13- CuOCuCl2	14- CuOCuCl2 2
Vapour Fraction		0.0000	0.2966	1.0000	0.0000	0.0000
Temperature	(C)	70.02	81.36	400.0 *	370.0 *	430.0 *
Pressure	(kPa)	50.00 *	50.00	50.00 *	50.00	101.3 *
Molar Flow	(kgmole/h)	4056.0	4056.0	4056.0	2028.0	2028.0
Mass Flow	(kg/h)	73069.2	73069.2	73069.2	433989	433989
Std Ideal Liq Vol Flow	(m3/h)	73.22	73.22	73.22	106.4	106.4
Heat Flow	(MW)	-318.526540	-303.531114	-257.557421	-192.535568	-188.022973
Molar Enthalpy	(kJ/kgmole)	-2.827e+005	-2.694e+005	-2.286e+005	-3.418e+005	-3.338e+005
Comp Mass Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Helium)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	1.0000	1.0000
Comp Mass Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (H2O)		1.0000	1.0000	1.0000	0.0000	0.0000
Comp Mass Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Helium)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	1.0000	1.0000
Comp Mole Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (H2O)		1.0000	1.0000	1.0000	0.0000	0.0000
Comp Mole Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000

Name		15- Oxygen	16- O2 cool	17- CuCl-L	18- CuCl cooled	19- HCl + H2O
Vapour Fraction		1.0000	1.0000	0.0000	0.0000	1.0000
Temperature	(C)	530.0 *	90.00 *	530.0	70.00 *	370.0
Pressure	(kPa)	101.3	101.3	101.3	2400 *	50.00
Molar Flow	(kgmole/h)	1014.0	1014.0	4056.0	4056.0	6084.0
Mass Flow	(kg/h)	32448.0	32448.0	401543	401543	184420
Std Ideal Liq Vol Flow	(m3/h)	28.52	28.52	96.99	96.99	206.5
Heat Flow	(MW)	4.48687984	0.538136166	-103.452445	-149.629912	-221.920712
Molar Enthalpy	(kJ/kgmole)	1.593e+004	1911	-9.182e+004	-1.328e+005	-1.313e+005
Comp Mass Frac (CuCl*)		0.0000	0.0000	1.0000	1.0000	0.0000
Comp Mass Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.8019
Comp Mass Frac (Helium)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (H2O)		0.0000	0.0000	0.0000	0.0000	0.1981
Comp Mass Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Oxygen)		1.0000	1.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl*)		0.0000	0.0000	1.0000	1.0000	0.0000
Comp Mole Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.6667
Comp Mole Frac (Helium)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (H2O)		0.0000	0.0000	0.0000	0.0000	0.3333
Comp Mole Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Oxygen)		1.0000	1.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000

* Specified by user.

Streams (continued)

Fluid Pkg: All

Name	20- Recycle 1	21- Recycle 2	22- Recycle 3	23- Recycle 4	24- Air
Vapour Fraction	1.0000	0.0000 *	0.0000	0.6812	1.0000
Temperature (C)	90.00 *	-95.85	-95.37	80.00 *	25.00 *
Pressure (kPa)	50.00	50.00 *	2400 *	2400	200.0 *
Molar Flow (kgmole/h)	6084.0	6084.0	6084.0	6084.0	11693
Mass Flow (kg/h)	184420	184420	184420	184420	336367
Std Ideal Liq Vol Flow (m3/h)	206.5	206.5	206.5	206.5	391.6
Heat Flow (MW)	-236.916139	-293.851810	-293.717206	-260.781606	-5.21336970e-002
Molar Enthalpy (kJ/kgmole)	-1.402e+005	-1.739e+005	-1.738e+005	-1.543e+005	-16.05
Comp Mass Frac (CuCl*)	0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (HCl)	0.8019	0.8019	0.8019	0.8019	0.0000 *
Comp Mass Frac (Helium)	0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (CuO.CuCl2*)	0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (CuCl2*)	0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (H2O)	0.1981	0.1981	0.1981	0.1981	0.0000 *
Comp Mass Frac (Hydrogen)	0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (Oxygen)	0.0000	0.0000	0.0000	0.0000	0.2100 *
Comp Mass Frac (Nitrogen)	0.0000	0.0000	0.0000	0.0000	0.7900 *
Comp Mole Frac (CuCl*)	0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (HCl)	0.6667	0.6667	0.6667	0.6667	0.0000 *
Comp Mole Frac (Helium)	0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (CuO.CuCl2*)	0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (CuCl2*)	0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (H2O)	0.3333	0.3333	0.3333	0.3333	0.0000 *
Comp Mole Frac (Hydrogen)	0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (Oxygen)	0.0000	0.0000	0.0000	0.0000	0.1888 *
Comp Mole Frac (Nitrogen)	0.0000	0.0000	0.0000	0.0000	0.8112 *

Name	25- Air	26 - Air	27- Air	30 - He	31- He in
Vapour Fraction	1.0000	1.0000	1.0000	1.0000	1.0000
Temperature (C)	490.0 *	390.0 *	126.5	720.8	720.8 *
Pressure (kPa)	200.0 *	200.0	200.0	3000	3000 *
Molar Flow (kgmole/h)	11693	11693	11693	2.8779e+005	1.4389e+005
Mass Flow (kg/h)	336367	336367	336367	1.15200e+006	576000
Std Ideal Liq Vol Flow (m3/h)	391.6	391.6	391.6	9286	4643
Heat Flow (MW)	46.1253333	35.8619542	9.68553038	1157.27972	578.639862
Molar Enthalpy (kJ/kgmole)	1.420e+004	1.104e+004	2982	1.448e+004	1.448e+004
Comp Mass Frac (CuCl*)	0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (HCl)	0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (Helium)	0.0000	0.0000	0.0000	1.0000	1.0000 *
Comp Mass Frac (CuO.CuCl2*)	0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (CuCl2*)	0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (H2O)	0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (Hydrogen)	0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (Oxygen)	0.2100	0.2100	0.2100	0.0000	0.0000 *
Comp Mass Frac (Nitrogen)	0.7900	0.7900	0.7900	0.0000	0.0000 *
Comp Mole Frac (CuCl*)	0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (HCl)	0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (Helium)	0.0000	0.0000	0.0000	1.0000	1.0000 *
Comp Mole Frac (CuO.CuCl2*)	0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (CuCl2*)	0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (H2O)	0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (Hydrogen)	0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (Oxygen)	0.1888	0.1888	0.1888	0.0000	0.0000 *
Comp Mole Frac (Nitrogen)	0.8112	0.8112	0.8112	0.0000	0.0000 *

* Specified by user.

Streams (continued)

Fluid Pkg: All

Name		32- He	33- He	34- He	35- He	36- He
Vapour Fraction		1.0000	1.0000	1.0000	1.0000	1.0000
Temperature	(C)	613.7	608.3	555.8	568.1	355.4
Pressure	(kPa)	3000	3000	3000	3000	3000
Molar Flow	(kgmole/h)	1.4389e+005	1.4389e+005	1.4389e+005	1.4389e+005	1.4389e+005
Mass Flow	(kg/h)	576000	576000	576000	576000	576000
Std Ideal Liq Vol Flow	(m3/h)	4643	4643	4643	4643	4643
Heat Flow	(MW)	489.582453	485.069858	441.400313	451.663692	274.702224
Molar Enthalpy	(kJ/kgmole)	1.225e+004	1.214e+004	1.104e+004	1.130e+004	6873
Comp Mass Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Helium)		1.0000	1.0000	1.0000	1.0000	1.0000
Comp Mass Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (H2O)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Helium)		1.0000	1.0000	1.0000	1.0000	1.0000
Comp Mole Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (H2O)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000

Name		37- He	40	41	Q air	Q extra H2O
Vapour Fraction		1.0000	1.0000	1.0000	---	---
Temperature	(C)	300.1	720.8	300.1	---	---
Pressure	(kPa)	3000	3000	3000	---	---
Molar Flow	(kgmole/h)	1.4389e+005	1.4389e+005	1.4389e+005	---	---
Mass Flow	(kg/h)	576000 *	576000	576000	---	---
Std Ideal Liq Vol Flow	(m3/h)	4643	4643	4643	---	---
Heat Flow	(MW)	228.728531	578.639862	228.728531	10.2633791	45.9736928
Molar Enthalpy	(kJ/kgmole)	5722	1.448e+004	5722	---	---
Comp Mass Frac (CuCl*)		0.0000	0.0000	0.0000	---	---
Comp Mass Frac (HCl)		0.0000	0.0000	0.0000	---	---
Comp Mass Frac (Helium)		1.0000	1.0000	1.0000	---	---
Comp Mass Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	---	---
Comp Mass Frac (CuCl2*)		0.0000	0.0000	0.0000	---	---
Comp Mass Frac (H2O)		0.0000	0.0000	0.0000	---	---
Comp Mass Frac (Hydrogen)		0.0000	0.0000	0.0000	---	---
Comp Mass Frac (Oxygen)		0.0000	0.0000	0.0000	---	---
Comp Mass Frac (Nitrogen)		0.0000	0.0000	0.0000	---	---
Comp Mole Frac (CuCl*)		0.0000	0.0000	0.0000	---	---
Comp Mole Frac (HCl)		0.0000	0.0000	0.0000	---	---
Comp Mole Frac (Helium)		1.0000	1.0000	1.0000	---	---
Comp Mole Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	---	---
Comp Mole Frac (CuCl2*)		0.0000	0.0000	0.0000	---	---
Comp Mole Frac (H2O)		0.0000	0.0000	0.0000	---	---
Comp Mole Frac (Hydrogen)		0.0000	0.0000	0.0000	---	---
Comp Mole Frac (Oxygen)		0.0000	0.0000	0.0000	---	---
Comp Mole Frac (Nitrogen)		0.0000	0.0000	0.0000	---	---

* Specified by user.

Streams (continued)

Fluid Pkg: All

Name		Q pump	Q-CuOCuCl2	Qdryer	Qe-needed	QNA1
Vapour Fraction		---	---	---	---	---
Temperature	(C)	---	---	---	---	---
Pressure	(kPa)	---	---	---	---	---
Molar Flow	(kgmole/h)	---	---	---	---	---
Mass Flow	(kg/h)	---	---	---	---	---
Std Ideal Liq Vol Flow	(m3/h)	---	---	---	---	---
Heat Flow	(MW)	0.134603682	4.51259485	24.8307760	176.961468 *	25.5918188
Molar Enthalpy	(kJ/kgmole)	---	---	---	---	---
Comp Mass Frac (CuCl*)		---	---	---	---	---
Comp Mass Frac (HCl)		---	---	---	---	---
Comp Mass Frac (Helium)		---	---	---	---	---
Comp Mass Frac (CuO.CuCl2*)		---	---	---	---	---
Comp Mass Frac (CuCl2*)		---	---	---	---	---
Comp Mass Frac (H2O)		---	---	---	---	---
Comp Mass Frac (Hydrogen)		---	---	---	---	---
Comp Mass Frac (Oxygen)		---	---	---	---	---
Comp Mass Frac (Nitrogen)		---	---	---	---	---
Comp Mole Frac (CuCl*)		---	---	---	---	---
Comp Mole Frac (HCl)		---	---	---	---	---
Comp Mole Frac (Helium)		---	---	---	---	---
Comp Mole Frac (CuO.CuCl2*)		---	---	---	---	---
Comp Mole Frac (CuCl2*)		---	---	---	---	---
Comp Mole Frac (H2O)		---	---	---	---	---
Comp Mole Frac (Hydrogen)		---	---	---	---	---
Comp Mole Frac (Oxygen)		---	---	---	---	---
Comp Mole Frac (Nitrogen)		---	---	---	---	---

Name		QNA2	QNA3	QR2	QR3	Qth
Vapour Fraction		---	---	---	---	---
Temperature	(C)	---	---	---	---	---
Pressure	(kPa)	---	---	---	---	---
Molar Flow	(kgmole/h)	---	---	---	---	---
Mass Flow	(kg/h)	---	---	---	---	---
Std Ideal Liq Vol Flow	(m3/h)	---	---	---	---	---
Heat Flow	(MW)	56.9356715	32.9356006	43.6695456	89.0574085	349.911331
Molar Enthalpy	(kJ/kgmole)	---	---	---	---	---
Comp Mass Frac (CuCl*)		---	---	---	---	---
Comp Mass Frac (HCl)		---	---	---	---	---
Comp Mass Frac (Helium)		---	---	---	---	---
Comp Mass Frac (CuO.CuCl2*)		---	---	---	---	---
Comp Mass Frac (CuCl2*)		---	---	---	---	---
Comp Mass Frac (H2O)		---	---	---	---	---
Comp Mass Frac (Hydrogen)		---	---	---	---	---
Comp Mass Frac (Oxygen)		---	---	---	---	---
Comp Mass Frac (Nitrogen)		---	---	---	---	---
Comp Mole Frac (CuCl*)		---	---	---	---	---
Comp Mole Frac (HCl)		---	---	---	---	---
Comp Mole Frac (Helium)		---	---	---	---	---
Comp Mole Frac (CuO.CuCl2*)		---	---	---	---	---
Comp Mole Frac (CuCl2*)		---	---	---	---	---
Comp Mole Frac (H2O)		---	---	---	---	---
Comp Mole Frac (Hydrogen)		---	---	---	---	---
Comp Mole Frac (Oxygen)		---	---	---	---	---
Comp Mole Frac (Nitrogen)		---	---	---	---	---

Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc Level
CRV-101	Conversion Reactor	12- H2O	13- CuOCuCl2	No	500.0 *

* Specified by user.

Unit Ops (continued)

Operation Name	Operation Type	Feeds	Products	Ignored	Calc Level
CRV-101	Conversion Reactor	6- CuCl2 hot QR2	19- HCl + H2O QR2	No	500.0 *
CRV-102	Conversion Reactor	14- CuOCuCl2 2 QR3	17- CuCl-L 15- Oxygen QR3	No	500.0 *
CRV-100	Conversion Reactor	1- HCl 2- CuCl QNA1	4- CuCl2 3- H2 QNA1	No	500.0 *
E-105	Cooler	31- He in	32- He QR3	No	500.0 *
E-108	Cooler	33- He	34- He QR2	No	500.0 *
E-109	Cooler	35- He	36- He Qe-needed	No	500.0 *
E-115	Cooler	32- He	33- He Q-CuOCuCl2	No	500.0 *
E-116	Cooler	20- Recycle 1	21- Recycle 2 QNA2	No	500.0 *
E-118	Cooler	36- He	37- He Q extra H2O	No	500.0 *
E-119	Cooler	40	41 Qth	No	500.0 *
E-110	Cooler	25- Air	26 - Air Q air	No	500.0 *
E-111	Heater	13- CuOCuCl2 Q-CuOCuCl2	14- CuOCuCl2 2	No	500.0 *
E-100	Heater	11- H2O 1 Q extra H2O	12- H2O	No	500.0 *
E-117	Heater	22- Recycle 3 QNA3	23- Recycle 4	No	500.0 *
E-112	Heater	34- He Q air	35- He	No	500.0 *
V-100	Tank	4- CuCl2 Qdryer	5- CuCl2 dry 7- H2O vap Qdryer	No	500.0 *
P-100	Pump	21- Recycle 2 Q pump	22- Recycle 3	No	500.0 *
SET-1	Set			No	500.0 *
SET-2	Set			No	500.0 *
SET-3	Set			No	500.0 *
SET-4	Set			No	500.0 *
TEE-100	Tee	30 - He	31- He in 40	No	500.0 *
E-104	Heat Exchanger	17- CuCl-L 24- Air	18- CuCl cooled 25- Air	No	500.0 *
E-103	Heat Exchanger	9- H2O cold 15- Oxygen	10 - H2O 16- O2 cool	No	500.0 *
E-101	Heat Exchanger	10 - H2O 19- HCl + H2O	11- H2O 1 20- Recycle 1	No	500.0 *
E-106	Heat Exchanger	5- CuCl2 dry 26 - Air	6- CuCl2 hot 27- Air	No	500.0 *
MIX-100	Mixer	8- H2O cold 8.1	9- H2O cold	No	500.0 *

Table A-3: Mass and Energy Balance for the Kemp Model

Streams

Fluid Pkg: All

Name		1- HCl	2- CuCl	3-H2	4- CuCl2	5- CuCl2 dry
Vapour Fraction		0.6756	0.0000	1.0000	0.0000	0.0000
Temperature	(C)	70.00 *	70.00 *	70.00	70.00 *	82.00
Pressure	(kPa)	2400 *	2400 *	2400	2400	50.00 *
Molar Flow	(kgmole/h)	6390.0	4260.0	2160.2	6359.9	4260.0
Mass Flow	(kg/h)	193695	421736	4840.42	610595	572769
Std Ideal Liq Vol Flow	(m3/h)	216.9	101.9	62.01	206.4	168.5
Heat Flow	(MW)	-275.156840	-157.154406	-1.26914522	-404.163113	-238.149154
Molar Enthalpy	(kJ/kgmole)	-1.550e+005	-1.328e+005	-2115	-2.288e+005	-2.013e+005
Comp Mass Frac (CuCl*)		0.0000 *	1.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (HCl)		0.8019 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (Helium)		0.0000 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (CuO.CuCl2*)		0.0000 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (CuCl2*)		0.0000 *	0.0000 *	0.0000	0.9380	1.0000
Comp Mass Frac (H2O)		0.1981 *	0.0000 *	0.1129	0.0619	0.0000
Comp Mass Frac (Hydrogen)		0.0000 *	0.0000 *	0.8871	0.0000	0.0000
Comp Mass Frac (Oxygen)		0.0000 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (Nitrogen)		0.0000 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl*)		0.0000 *	1.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (HCl)		0.6667 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (Helium)		0.0000 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (CuO.CuCl2*)		0.0000 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl2*)		0.0000 *	0.0000 *	0.0000	0.6698	1.0000
Comp Mole Frac (H2O)		0.3333 *	0.0000 *	0.0140	0.3301	0.0000
Comp Mole Frac (Hydrogen)		0.0000 *	0.0000 *	0.9860	0.0000	0.0000
Comp Mole Frac (Oxygen)		0.0000 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (Nitrogen)		0.0000 *	0.0000 *	0.0000	0.0000	0.0000

Name		6- CuCl2 dry	7- CuCl2 hot	7- H2O Vap	8- Water	9
Vapour Fraction		0.0000	0.0000	1.0000	0.0000	1.0000
Temperature	(C)	110.6	370.0 *	82.00 *	25.00 *	250.0 *
Pressure	(kPa)	50.00	50.00	50.00 *	101.3 *	50.00 *
Molar Flow	(kgmole/h)	4260.0	4260.0	2099.8	4260.0 *	4260.0
Mass Flow	(kg/h)	572769	572769	37825.8	76744.3	76744.3
Std Ideal Liq Vol Flow	(m3/h)	168.5	168.5	37.91	76.90	76.90
Heat Flow	(MW)	-235.415097	-210.656165	-139.934297	-338.694455	-276.993700
Molar Enthalpy	(kJ/kgmole)	-1.989e+005	-1.780e+005	-2.399e+005	-2.862e+005	-2.341e+005
Comp Mass Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (HCl)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (Helium)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (CuCl2*)		1.0000	1.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (H2O)		0.0000	0.0000	1.0000	1.0000 *	1.0000
Comp Mass Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (HCl)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (Helium)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (CuCl2*)		1.0000	1.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (H2O)		0.0000	0.0000	0.9999	1.0000 *	1.0000
Comp Mole Frac (Hydrogen)		0.0000	0.0000	0.0001	0.0000 *	0.0000
Comp Mole Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000 *	0.0000

* Specified by user.

Streams (continued)

Fluid Pkg: All

Name		10- H2O	11- CuOCuCl2	12- CuOCuCl2	13- CuOCuCl2	14- Oxygen
Vapour Fraction		1.0000	0.0000	0.0000	0.0000	1.0000
Temperature	(C)	400.0 *	370.0 *	388.0 *	430.0 *	530.0 *
Pressure	(kPa)	50.00 *	50.00	101.3 *	101.3	101.3
Molar Flow	(kgmole/h)	4260.0	2130.0	2130.0	2130.0	1065.0
Mass Flow	(kg/h)	76744.3	455817	455817	455817	34080.0
Std Ideal Liq Vol Flow	(m3/h)	76.90	111.7	111.7	111.7	29.96
Heat Flow	(MW)	-270.511492	-202.219310	-200.806018	-197.479750	4.71255131
Molar Enthalpy	(kJ/kgmole)	-2.286e+005	-3.418e+005	-3.394e+005	-3.338e+005	1.593e+004
Comp Mass Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Helium)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuO.CuCl2*)		0.0000	1.0000	1.0000	1.0000	0.0000
Comp Mass Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (H2O)		1.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	1.0000
Comp Mass Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Helium)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuO.CuCl2*)		0.0000	1.0000	1.0000	1.0000	0.0000
Comp Mole Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (H2O)		1.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	1.0000
Comp Mole Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000

Name		15- O2 cool	16- O2 cool	17- CuCl-l	18- CuCl cooled	19- HCl + H2O
Vapour Fraction		1.0000	1.0000	0.0000	0.0000	1.0000
Temperature	(C)	385.8	90.00 *	530.0	70.00 *	370.0
Pressure	(kPa)	101.3	101.3	101.3	2400 *	50.00
Molar Flow	(kgmole/h)	1065.0	1065.0	4260.0	4260.0	6390.0
Mass Flow	(kg/h)	34080.0	34080.0	421739	421739	193695
Std Ideal Liq Vol Flow	(m3/h)	29.96	29.96	101.9	101.9	216.9
Heat Flow	(MW)	3.29925977	0.565202186	-108.655674	-157.155676	-233.082405
Molar Enthalpy	(kJ/kgmole)	1.115e+004	1911	-9.182e+004	-1.328e+005	-1.313e+005
Comp Mass Frac (CuCl*)		0.0000	0.0000	1.0000	1.0000	0.0000
Comp Mass Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.8019
Comp Mass Frac (Helium)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (H2O)		0.0000	0.0000	0.0000	0.0000	0.1981
Comp Mass Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Oxygen)		1.0000	1.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl*)		0.0000	0.0000	1.0000	1.0000	0.0000
Comp Mole Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.6667
Comp Mole Frac (Helium)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (H2O)		0.0000	0.0000	0.0000	0.0000	0.3333
Comp Mole Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Oxygen)		1.0000	1.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000

Streams (continued)

Fluid Pkg: All

Name		20	21- HCl + H2O recycle	22	23- HCl + H2O Recycle	24- Air
Vapour Fraction		0.7834	1.0000	0.0000 *	0.0000	1.0000
Temperature	(C)	40.30	70.00 *	-95.85	-95.37	25.00 *
Pressure	(kPa)	50.00	50.00 *	50.00	2400 *	200.0 *
Molar Flow	(kgmole/h)	6390.0	6390.0	6390.0	6390.0	21300
Mass Flow	(kg/h)	193695	193695	193695	193695	612702
Std Ideal Liq Vol Flow	(m3/h)	216.9	216.9	216.9	216.9	713.4
Heat Flow	(MW)	-268.368569	-249.935546	-308.631339	-308.489965	-9.49629203e-002
Molar Enthalpy	(kJ/kgmole)	-1.512e+005	-1.408e+005	-1.739e+005	-1.738e+005	-16.05
Comp Mass Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (HCl)		0.8019	0.8019	0.8019	0.8019	0.0000 *
Comp Mass Frac (Helium)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (H2O)		0.1981	0.1981	0.1981	0.1981	0.0000 *
Comp Mass Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	0.2100 *
Comp Mass Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.7900 *
Comp Mole Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (HCl)		0.6667	0.6667	0.6667	0.6667	0.0000 *
Comp Mole Frac (Helium)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (H2O)		0.3333	0.3333	0.3333	0.3333	0.0000 *
Comp Mole Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	0.1888 *
Comp Mole Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.8112 *

Name		25- Air	26- Air	26-Air	27- Air	28- Air
Vapour Fraction		1.0000	1.0000	1.0000	1.0000	1.0000
Temperature	(C)	225.0 *	25.00 *	490.0 *	459.3	399.1
Pressure	(kPa)	200.0	200.0 *	200.0	200.0	200.0
Molar Flow	(kgmole/h)	21300	12281	12281	12281	12281
Mass Flow	(kg/h)	612702	353285	353285	353285	353285
Std Ideal Liq Vol Flow	(m3/h)	713.4	411.3	411.3	411.3	411.3
Heat Flow	(MW)	35.1912010	-5.47558061e-002	48.4452466	45.1189784	38.6367709
Molar Enthalpy	(kJ/kgmole)	5948	-16.05	1.420e+004	1.323e+004	1.133e+004
Comp Mass Frac (CuCl*)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (HCl)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (Helium)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (CuO.CuCl2*)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (CuCl2*)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (H2O)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (Hydrogen)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (Oxygen)		0.2100	0.2100 *	0.2100	0.2100	0.2100
Comp Mass Frac (Nitrogen)		0.7900	0.7900 *	0.7900	0.7900	0.7900
Comp Mole Frac (CuCl*)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (HCl)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (Helium)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (CuO.CuCl2*)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl2*)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (H2O)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (Hydrogen)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (Oxygen)		0.1888	0.1888 *	0.1888	0.1888	0.1888
Comp Mole Frac (Nitrogen)		0.8112	0.8112 *	0.8112	0.8112	0.8112

Streams (continued)

Fluid Pkg: All

Name		29- Air	30- Air recycle	40- He In	41- He	42- He
Vapour Fraction		1.0000	1.0000	1.0000	1.0000	1.0000
Temperature	(C)	289.3	69.80	720.8 *	720.8	439.6
Pressure	(kPa)	200.0	200.0	3000 *	3000	3000
Molar Flow	(kgmole/h)	33581	33581	1.4389e+005	57557	57557
Mass Flow	(kg/h)	965987	965987	576000 *	230400	230400
Std Ideal Liq Vol Flow	(m3/h)	1125	1125	4643	1857	1857
Heat Flow	(MW)	73.8279719	12.1272167	578.639862	231.455945	137.919317
Molar Enthalpy	(kJ/kgmole)	7915	1300	1.448e+004	1.448e+004	8626
Comp Mass Frac (CuCl*)		0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mass Frac (HCl)		0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mass Frac (Helium)		0.0000	0.0000	1.0000 *	1.0000	1.0000
Comp Mass Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mass Frac (CuCl2*)		0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mass Frac (H2O)		0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mass Frac (Hydrogen)		0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mass Frac (Oxygen)		0.2100	0.2100	0.0000 *	0.0000	0.0000
Comp Mass Frac (Nitrogen)		0.7900	0.7900	0.0000 *	0.0000	0.0000
Comp Mole Frac (CuCl*)		0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mole Frac (HCl)		0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mole Frac (Helium)		0.0000	0.0000	1.0000 *	1.0000	1.0000
Comp Mole Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mole Frac (CuCl2*)		0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mole Frac (H2O)		0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mole Frac (Hydrogen)		0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mole Frac (Oxygen)		0.1888	0.1888	0.0000 *	0.0000	0.0000
Comp Mole Frac (Nitrogen)		0.8112	0.8112	0.0000 *	0.0000	0.0000

Name		43- He	44- He	45- He for electricity	46- He	47- He Out
Vapour Fraction		1.0000	1.0000	1.0000	1.0000	1.0000
Temperature	(C)	301.8	227.4	720.8	348.4	300.0
Pressure	(kPa)	3000	3000	3000	3000	3000
Molar Flow	(kgmole/h)	57557	57557	86336	86336	1.4389e+005
Mass Flow	(kg/h)	230400	230400	345600	345600	576000
Std Ideal Liq Vol Flow	(m3/h)	1857	1857	2786	2786	4643
Heat Flow	(MW)	92.0533745	67.2944426	347.183917	161.323917	228.618360
Molar Enthalpy	(kJ/kgmole)	5758	4209	1.448e+004	6727	5720
Comp Mass Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Helium)		1.0000	1.0000	1.0000	1.0000	1.0000
Comp Mass Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (H2O)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Helium)		1.0000	1.0000	1.0000	1.0000	1.0000
Comp Mole Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (H2O)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000

Streams (continued)

Fluid Pkg: All

Name		50	51	52	Q CuCl2 heat	Q pump
Vapour Fraction		1.0000	1.0000	1.0000	---	---
Temperature	(C)	720.8	720.8	300.0	---	---
Pressure	(kPa)	3000	3000	3000	---	---
Molar Flow	(kgmole/h)	2.8779e+005	1.4389e+005	1.4389e+005	---	---
Mass Flow	(kg/h)	1.15200e+006	576000	576000	---	---
Std Ideal Liq Vol Flow	(m3/h)	9286	4643	4643	---	---
Heat Flow	(MW)	1157.27972	578.639862	228.618360	24.7589319	0.141373689
Molar Enthalpy	(kJ/kgmole)	1.448e+004	1.448e+004	5720	---	---
Comp Mass Frac (CuCl*)		0.0000	0.0000	0.0000	---	---
Comp Mass Frac (HCl)		0.0000	0.0000	0.0000	---	---
Comp Mass Frac (Helium)		1.0000	1.0000	1.0000	---	---
Comp Mass Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	---	---
Comp Mass Frac (CuCl2*)		0.0000	0.0000	0.0000	---	---
Comp Mass Frac (H2O)		0.0000	0.0000	0.0000	---	---
Comp Mass Frac (Hydrogen)		0.0000	0.0000	0.0000	---	---
Comp Mass Frac (Oxygen)		0.0000	0.0000	0.0000	---	---
Comp Mass Frac (Nitrogen)		0.0000	0.0000	0.0000	---	---
Comp Mole Frac (CuCl*)		0.0000	0.0000	0.0000	---	---
Comp Mole Frac (HCl)		0.0000	0.0000	0.0000	---	---
Comp Mole Frac (Helium)		1.0000	1.0000	1.0000	---	---
Comp Mole Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	---	---
Comp Mole Frac (CuCl2*)		0.0000	0.0000	0.0000	---	---
Comp Mole Frac (H2O)		0.0000	0.0000	0.0000	---	---
Comp Mole Frac (Hydrogen)		0.0000	0.0000	0.0000	---	---
Comp Mole Frac (Oxygen)		0.0000	0.0000	0.0000	---	---
Comp Mole Frac (Nitrogen)		0.0000	0.0000	0.0000	---	---

Name		Q waste extra	Qdryer	Qe-needed	QNA1	QNA2
Vapour Fraction		---	---	---	---	---
Temperature	(C)	---	---	---	---	---
Pressure	(kPa)	---	---	---	---	---
Molar Flow	(kgmole/h)	---	---	---	---	---
Mass Flow	(kg/h)	---	---	---	---	---
Std Ideal Liq Vol Flow	(m3/h)	---	---	---	---	---
Heat Flow	(MW)	18.4330230	26.0796612	185.860000 *	26.8789813	58.6957935
Molar Enthalpy	(kJ/kgmole)	---	---	---	---	---
Comp Mass Frac (CuCl*)		---	---	---	---	---
Comp Mass Frac (HCl)		---	---	---	---	---
Comp Mass Frac (Helium)		---	---	---	---	---
Comp Mass Frac (CuO.CuCl2*)		---	---	---	---	---
Comp Mass Frac (CuCl2*)		---	---	---	---	---
Comp Mass Frac (H2O)		---	---	---	---	---
Comp Mass Frac (Hydrogen)		---	---	---	---	---
Comp Mass Frac (Oxygen)		---	---	---	---	---
Comp Mass Frac (Nitrogen)		---	---	---	---	---
Comp Mole Frac (CuCl*)		---	---	---	---	---
Comp Mole Frac (HCl)		---	---	---	---	---
Comp Mole Frac (Helium)		---	---	---	---	---
Comp Mole Frac (CuO.CuCl2*)		---	---	---	---	---
Comp Mole Frac (CuCl2*)		---	---	---	---	---
Comp Mole Frac (H2O)		---	---	---	---	---
Comp Mole Frac (Hydrogen)		---	---	---	---	---
Comp Mole Frac (Oxygen)		---	---	---	---	---
Comp Mole Frac (Nitrogen)		---	---	---	---	---

* Specified by user.

Streams (continued)

Fluid Pkg: All

Name		QR2	QR3	Qth		
Vapour Fraction		---	---	---		
Temperature	(C)	---	---	---		
Pressure	(kPa)	---	---	---		
Molar Flow	(kgmole/h)	---	---	---		
Mass Flow	(kg/h)	---	---	---		
Std Ideal Liq Vol Flow	(m3/h)	---	---	---		
Heat Flow	(MW)	45.8659429	93.5366272	350.021502		
Molar Enthalpy	(kJ/kgmole)	---	---	---		
Comp Mass Frac (CuCl*)		---	---	---		
Comp Mass Frac (HCl)		---	---	---		
Comp Mass Frac (Helium)		---	---	---		
Comp Mass Frac (CuO.CuCl2*)		---	---	---		
Comp Mass Frac (CuCl2*)		---	---	---		
Comp Mass Frac (H2O)		---	---	---		
Comp Mass Frac (Hydrogen)		---	---	---		
Comp Mass Frac (Oxygen)		---	---	---		
Comp Mass Frac (Nitrogen)		---	---	---		
Comp Mole Frac (CuCl*)		---	---	---		
Comp Mole Frac (HCl)		---	---	---		
Comp Mole Frac (Helium)		---	---	---		
Comp Mole Frac (CuO.CuCl2*)		---	---	---		
Comp Mole Frac (CuCl2*)		---	---	---		
Comp Mole Frac (H2O)		---	---	---		
Comp Mole Frac (Hydrogen)		---	---	---		
Comp Mole Frac (Oxygen)		---	---	---		
Comp Mole Frac (Nitrogen)		---	---	---		

Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc Level
CRV-101	Conversion Reactor	10- H2O	11- CuOCuCl2	No	500.0 *
		7- CuCl2 hot	19- HCl + H2O		
		QR2	QR2		
CRV-102	Conversion Reactor	13- CuOCuCl2	17- CuCl-l	No	500.0 *
		QR3	14- Oxygen		
			QR3		
CRV-100	Conversion Reactor	1- HCl	4- CuCl2	No	500.0 *
		2- CuCl	3-H2		
		QNA1	QNA1		
E-105	Cooler	41- He	42- He	No	500.0 *
			QR3		
E-108	Cooler	43- He	44- He	No	500.0 *
			Q CuCl2 heat		
E-109	Cooler	45- He for electricity	46- He	No	500.0 *
			Qe-needed		
E-112	Cooler	42- He	43- He	No	500.0 *
			QR2		
E-111	Cooler	51	52	No	500.0 *
			Qth		
E-107	Cooler	21- HCl + H2O recycle	22	No	500.0 *
			QNA2		
E-106	Heater	6- CuCl2 dry	7- CuCl2 hot	No	500.0 *
		Q CuCl2 heat			
E-102	Heater	20	21- HCl + H2O recycle	No	500.0 *
		Q waste extra			
V-100	Tank	4- CuCl2	5- CuCl2 dry	No	500.0 *
		Qdryer	7- H2O Vap		
			Qdryer		

Unit Ops (continued)

Operation Name	Operation Type	Feeds	Products	Ignored	Calc Level
E-101	Heat Exchanger	11- CuOCuCl2	12- CuOCuCl2	No	500.0 *
		14- Oxygen	15- O2 cool		
E-104	Heat Exchanger	17- CuCl-l	18- CuCl cooled	No	500.0 *
		26- Air	26-Air		
E-103	Heat Exchanger	12- CuOCuCl2	13- CuOCuCl2	No	500.0 *
		26-Air	27- Air		
E-100	Heat Exchanger	9	10- H2O	No	500.0 *
		27- Air	28- Air		
E-110	Heat Exchanger	19- HCl + H2O	20	No	500.0 *
		24- Air	25- Air		
E-114	Heat Exchanger	29- Air	30- Air recycle	No	500.0 *
		8- Water	9		
E-115	Heat Exchanger	5- CuCl2 dry	6- CuCl2 dry	No	500.0 *
		15- O2 cool	16- O2 cool		
MIX-101	Mixer	25- Air	29- Air	No	500.0 *
		28- Air			
MIX-100	Mixer	44- He	47- He Out	No	500.0 *
		46- He			
TEE-100	Tee	50	40- He In	No	500.0 *
			51		
TEE-101	Tee	40- He In	41- He	No	500.0 *
			45- He for electricity		
SET-3	Set			No	500.0 *
SET-2	Set			No	500.0 *
SET-1	Set			No	500.0 *
SET-4	Set			No	500.0 *
P-100	Pump	22	23- HCl + H2O Recycle	No	500.0 *
		Q pump			

Table A-4: Mass and Energy Balance for the Excess Model

Streams Fluid Pkg: All

Name		1- HCl	1.1 Equavalent water	1.2	2- CuCl	3-H2
Vapour Fraction		0.6756	0.0000	0.1487	0.0000	1.0000
Temperature	(C)	70.00 *	70.00 *	69.84	70.00 *	70.00
Pressure	(kPa)	2400 *	2400 *	2400	2400 *	2400
Molar Flow	(kgmole/h)	6096.0	20625	26721	4064.0	2059.1
Mass Flow	(kg/h)	184783	371558	556341	402332	4613.85
Std Ideal Liq Vol Flow	(m3/h)	206.9	372.3	579.2	97.18	59.11
Heat Flow	(MW)	-262.497042	-1619.50562	-1882.00266	-149.923828	-1.20973889
Molar Enthalpy	(kJ/kgmole)	-1.550e+005	-2.827e+005	-2.536e+005	-1.328e+005	-2115
Comp Mass Frac (CuCl*)		0.0000 *	0.0000 *	0.0000	1.0000 *	0.0000
Comp Mass Frac (HCl)		0.8019 *	0.0000 *	0.2663	0.0000 *	0.0000
Comp Mass Frac (Helium)		0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
Comp Mass Frac (CuO.CuCl2*)		0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
Comp Mass Frac (CuCl2*)		0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
Comp Mass Frac (H2O)		0.1981 *	1.0000 *	0.7337	0.0000 *	0.1129
Comp Mass Frac (Hydrogen)		0.0000 *	0.0000 *	0.0000	0.0000 *	0.8871
Comp Mass Frac (Oxygen)		0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
Comp Mass Frac (Nitrogen)		0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
Comp Mole Frac (CuCl*)		0.0000 *	0.0000 *	0.0000	1.0000 *	0.0000
Comp Mole Frac (HCl)		0.6667 *	0.0000 *	0.1521	0.0000 *	0.0000
Comp Mole Frac (Helium)		0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
Comp Mole Frac (CuO.CuCl2*)		0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
Comp Mole Frac (CuCl2*)		0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
Comp Mole Frac (H2O)		0.3333 *	1.0000 *	0.8479	0.0000 *	0.0140
Comp Mole Frac (Hydrogen)		0.0000 *	0.0000 *	0.0000	0.0000 *	0.9860
Comp Mole Frac (Oxygen)		0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000
Comp Mole Frac (Nitrogen)		0.0000 *	0.0000 *	0.0000	0.0000 *	0.0000

Name		4- CuCl2	5- CuCl2 dry	6- CuCl2 hot	7- H2O Vap	8- H2O Cold
Vapour Fraction		0.0000	0.0000	0.0000	1.0000	0.0000
Temperature	(C)	70.00 *	82.00	370.0 *	82.00 *	25.00 *
Pressure	(kPa)	2400	50.00 *	50.00	50.00 *	101.3 *
Molar Flow	(kgmole/h)	26694	4064.0	4064.0	22630	2032.0 *
Mass Flow	(kg/h)	954063	546416	546416	407647	36606.7
Std Ideal Liq Vol Flow	(m3/h)	569.2	160.7	160.7	408.5	36.68
Heat Flow	(MW)	-2005.06450	-227.192057	-200.964003	-1508.06571	-161.555665
Molar Enthalpy	(kJ/kgmole)	-2.704e+005	-2.013e+005	-1.780e+005	-2.399e+005	-2.862e+005
Comp Mass Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (Helium)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (CuCl2*)		0.5727	1.0000	1.0000	0.0000	0.0000 *
Comp Mass Frac (H2O)		0.4273	0.0000	0.0000	1.0000	1.0000 *
Comp Mass Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (Helium)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (CuCl2*)		0.1522	1.0000	1.0000	0.0000	0.0000 *
Comp Mole Frac (H2O)		0.8477	0.0000	0.0000	0.9999	1.0000 *
Comp Mole Frac (Hydrogen)		0.0001	0.0000	0.0000	0.0001	0.0000 *
Comp Mole Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000 *

Streams (continued)

Fluid Pkg: All

Name		8.1	8.2	9- H2O Cold 0	10- H2O	11 - CuOCuCl2
Vapour Fraction		0.0000	0.0000	0.0248	1.0000	0.0000
Temperature	(C)	25.00 *	25.00	99.96	400.0 *	370.0 *
Pressure	(kPa)	101.3 *	101.3	101.3	50.00 *	50.00
Molar Flow	(kgmole/h)	304.80	2336.8	2336.8	2336.8	2032.0
Mass Flow	(kg/h)	5491.00	42097.7	42097.7	42097.7	434845
Std Ideal Liq Vol Flow	(m3/h)	5.502	42.18	42.18	42.18	106.6
Heat Flow	(MW)	-24.2333497	-185.789015	-181.324923	-148.387619	-192.915323
Molar Enthalpy	(kJ/kgmole)	-2.862e+005	-2.862e+005	-2.793e+005	-2.286e+005	-3.418e+005
Comp Mass Frac (CuCl*)		0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (HCl)		0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Helium)		0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuO.CuCl2*)		0.0000 *	0.0000	0.0000	0.0000	1.0000
Comp Mass Frac (CuCl2*)		0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (H2O)		1.0000 *	1.0000	1.0000	1.0000	0.0000
Comp Mass Frac (Hydrogen)		0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Oxygen)		0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Nitrogen)		0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl*)		0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (HCl)		0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Helium)		0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuO.CuCl2*)		0.0000 *	0.0000	0.0000	0.0000	1.0000
Comp Mole Frac (CuCl2*)		0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (H2O)		1.0000 *	1.0000	1.0000	1.0000	0.0000
Comp Mole Frac (Hydrogen)		0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Oxygen)		0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Nitrogen)		0.0000 *	0.0000	0.0000	0.0000	0.0000

Name		12 - CuOCuCl2	13- Oxygen	14- O2 cool	15- CuCl.l	16- CuCl cooled
Vapour Fraction		0.0000	1.0000	1.0000	0.0000	0.0000
Temperature	(C)	430.0 *	530.0 *	29.00 *	530.0	70.00 *
Pressure	(kPa)	50.00	50.00	50.00	50.00	2400 *
Molar Flow	(kgmole/h)	2032.0	1016.0	1016.0	4064.0	4064.0
Mass Flow	(kg/h)	434845	32512.0	32512.0	402335	402335
Std Ideal Liq Vol Flow	(m3/h)	106.6	28.58	28.58	97.18	97.18
Heat Flow	(MW)	-188.393827	4.49573926	3.16472786e-002	-103.656493	-149.925040
Molar Enthalpy	(kJ/kgmole)	-3.338e+005	1.593e+004	112.1	-9.182e+004	-1.328e+005
Comp Mass Frac (CuCl*)		0.0000	0.0000	0.0000	1.0000	1.0000
Comp Mass Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Helium)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuO.CuCl2*)		1.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (H2O)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Oxygen)		0.0000	1.0000	1.0000	0.0000	0.0000
Comp Mass Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl*)		0.0000	0.0000	0.0000	1.0000	1.0000
Comp Mole Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Helium)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuO.CuCl2*)		1.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (H2O)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Oxygen)		0.0000	1.0000	1.0000	0.0000	0.0000
Comp Mole Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000

* Specified by user.

Streams (continued)

Fluid Pkg: All

Name	17- Air	18- Air	19- Air	20- Air	21
Vapour Fraction	1.0000	1.0000	1.0000	1.0000	1.0000
Temperature (C)	25.00 *	490.0 *	446.2	116.7	35.00 *
Pressure (kPa)	200.0 *	200.0	200.0	200.0	200.0
Molar Flow (kgmole/h)	11716	11716	11716	11716	11716
Mass Flow (kg/h)	337031	337031	337031	337031	337031
Std Ideal Liq Vol Flow (m3/h)	392.4	392.4	392.4	392.4	392.4
Heat Flow (MW)	-5.22365248e-002	46.2163103	41.6948149	8.75751080	0.900681747
Molar Enthalpy (kJ/kgmole)	-16.05	1.420e+004	1.281e+004	2691	276.7
Comp Mass Frac (CuCl*)	0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (HCl)	0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Helium)	0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuO.CuCl2*)	0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuCl2*)	0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (H2O)	0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Hydrogen)	0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Oxygen)	0.2100 *	0.2100	0.2100	0.2100	0.2100
Comp Mass Frac (Nitrogen)	0.7900 *	0.7900	0.7900	0.7900	0.7900
Comp Mole Frac (CuCl*)	0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (HCl)	0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Helium)	0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuO.CuCl2*)	0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl2*)	0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (H2O)	0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Hydrogen)	0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Oxygen)	0.1888 *	0.1888	0.1888	0.1888	0.1888
Comp Mole Frac (Nitrogen)	0.8112 *	0.8112	0.8112	0.8112	0.8112

Name	22- HCl + H2O	23	24	24.1	25
Vapour Fraction	1.0000	0.2210	0.2181	0.0000	0.0000
Temperature (C)	370.0	54.86	54.26	-100.0 *	-99.83
Pressure (kPa)	50.00	50.00	50.00	50.00	2400 *
Molar Flow (kgmole/h)	26721	26721	26721	26721	26721
Mass Flow (kg/h)	556341	556341	556341	556341	556341
Std Ideal Liq Vol Flow (m3/h)	579.2	579.2	579.2	579.2	579.2
Heat Flow (MW)	-1538.44000	-1867.99085	-1869.19767	-1991.57036	-1991.14127
Molar Enthalpy (kJ/kgmole)	-2.073e+005	-2.517e+005	-2.518e+005	-2.683e+005	-2.683e+005
Comp Mass Frac (CuCl*)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (HCl)	0.2663	0.2663	0.2663	0.2663	0.2663
Comp Mass Frac (Helium)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuO.CuCl2*)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuCl2*)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (H2O)	0.7337	0.7337	0.7337	0.7337	0.7337
Comp Mass Frac (Hydrogen)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Oxygen)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Nitrogen)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl*)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (HCl)	0.1521	0.1521	0.1521	0.1521	0.1521
Comp Mole Frac (Helium)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuO.CuCl2*)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl2*)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (H2O)	0.8479	0.8479	0.8479	0.8479	0.8479
Comp Mole Frac (Hydrogen)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Oxygen)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Nitrogen)	0.0000	0.0000	0.0000	0.0000	0.0000

Streams (continued)

Fluid Pkg: All

Name		26- Extra water	27	28	29	30
Vapour Fraction		0.0000	0.0000	0.0000	0.0000	0.0000
Temperature	(C)	25.00 *	25.00	43.09	25.00	50.00 *
Pressure	(kPa)	101.3 *	101.3	101.3	101.3	101.3
Molar Flow	(kgmole/h)	22352	20117	20117	2235.2	2235.2
Mass Flow	(kg/h)	402674	362406	362406	40267.4	40267.4
Std Ideal Liq Vol Flow	(m3/h)	403.5	363.1	363.1	40.35	40.35
Heat Flow	(MW)	-1777.11231	-1599.40108	-1591.54425	-177.711231	-176.504408
Molar Enthalpy	(kJ/kgmole)	-2.862e+005	-2.862e+005	-2.848e+005	-2.862e+005	-2.843e+005
Comp Mass Frac (CuCl*)		0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (HCl)		0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Helium)		0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuO.CuCl2*)		0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuCl2*)		0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (H2O)		1.0000 *	1.0000	1.0000	1.0000	1.0000
Comp Mass Frac (Hydrogen)		0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Oxygen)		0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Nitrogen)		0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl*)		0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (HCl)		0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Helium)		0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuO.CuCl2*)		0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl2*)		0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (H2O)		1.0000 *	1.0000	1.0000	1.0000	1.0000
Comp Mole Frac (Hydrogen)		0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Oxygen)		0.0000 *	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Nitrogen)		0.0000 *	0.0000	0.0000	0.0000	0.0000

Name		31	32	33- Hot Extra Water	40 - Helium	41- He
Vapour Fraction		0.0000	1.0000	1.0000	1.0000	1.0000
Temperature	(C)	43.78	317.0 *	400.0 *	720.8	720.8 *
Pressure	(kPa)	101.3	101.3	101.3	3000	3000 *
Molar Flow	(kgmole/h)	22352	22352	22352	1.4389e+005	71946
Mass Flow	(kg/h)	402674	402674	402674	576000 *	288000
Std Ideal Liq Vol Flow	(m3/h)	403.5	403.5	403.5	4643	2321
Heat Flow	(MW)	-1768.04866	-1438.49781	-1419.44978	578.639862	289.319931
Molar Enthalpy	(kJ/kgmole)	-2.848e+005	-2.317e+005	-2.286e+005	1.448e+004	1.448e+004
Comp Mass Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (Helium)		0.0000	0.0000	0.0000	1.0000	1.0000 *
Comp Mass Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (H2O)		1.0000	1.0000	1.0000	0.0000	0.0000 *
Comp Mass Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (Helium)		0.0000	0.0000	0.0000	1.0000	1.0000 *
Comp Mole Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (H2O)		1.0000	1.0000	1.0000	0.0000	0.0000 *
Comp Mole Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000 *

Streams (continued)

Fluid Pkg: All

Name		42- He	43- He	44- He	45- He	46- He
Vapour Fraction		1.0000	1.0000	1.0000	1.0000	1.0000
Temperature	(C)	506.2	416.2	353.1	307.3	720.8
Pressure	(kPa)	3000	3000	3000	3000	3000
Molar Flow	(kgmole/h)	71946	71946	71946	71946	71946
Mass Flow	(kg/h)	288000	288000	288000	288000	288000
Std Ideal Liq Vol Flow	(m3/h)	2321	2321	2321	2321	2321
Heat Flow	(MW)	200.086857	162.640777	136.412723	117.364690	289.319931
Molar Enthalpy	(kJ/kgmole)	1.001e+004	8138	6826	5873	1.448e+004
Comp Mass Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Helium)		1.0000	1.0000	1.0000	1.0000	1.0000
Comp Mass Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (H2O)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Helium)		1.0000	1.0000	1.0000	1.0000	1.0000
Comp Mole Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (H2O)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000

Name		47- He	48-He out	50 - He big	51 He side	52- He side
Vapour Fraction		1.0000	1.0000	1.0000	1.0000	1.0000
Temperature	(C)	292.7	300.0	720.8	720.8	300.0
Pressure	(kPa)	3000	3000	3000	3000	3000
Molar Flow	(kgmole/h)	71946	1.4389e+005	2.8779e+005	1.4389e+005	1.4389e+005
Mass Flow	(kg/h)	288000	576000	1.15200e+006	576000	576000
Std Ideal Liq Vol Flow	(m3/h)	2321	4643	9286	4643	4643
Heat Flow	(MW)	111.269931	228.634621	1157.27972	578.639862	228.634621
Molar Enthalpy	(kJ/kgmole)	5568	5720	1.448e+004	1.448e+004	5720
Comp Mass Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Helium)		1.0000	1.0000	1.0000	1.0000	1.0000
Comp Mass Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (H2O)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Helium)		1.0000	1.0000	1.0000	1.0000	1.0000
Comp Mole Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (H2O)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000

Streams (continued)

Fluid Pkg: All

Name		Q CuCl2 heat	Q extra heat	Q NA	Q NA2	Q pump
Vapour Fraction		---	---	---	---	---
Temperature	(C)	---	---	---	---	---
Pressure	(kPa)	---	---	---	---	---
Molar Flow	(kgmole/h)	---	---	---	---	---
Mass Flow	(kg/h)	---	---	---	---	---
Std Ideal Liq Vol Flow	(m3/h)	---	---	---	---	---
Heat Flow	(MW)	26.2280539	19.0480330	25.6522426	122.372691	0.429094739
Molar Enthalpy	(kJ/kgmole)	---	---	---	---	---
Comp Mass Frac (CuCl*)		---	---	---	---	---
Comp Mass Frac (HCl)		---	---	---	---	---
Comp Mass Frac (Helium)		---	---	---	---	---
Comp Mass Frac (CuO.CuCl2*)		---	---	---	---	---
Comp Mass Frac (CuCl2*)		---	---	---	---	---
Comp Mass Frac (H2O)		---	---	---	---	---
Comp Mass Frac (Hydrogen)		---	---	---	---	---
Comp Mass Frac (Oxygen)		---	---	---	---	---
Comp Mass Frac (Nitrogen)		---	---	---	---	---
Comp Mole Frac (CuCl*)		---	---	---	---	---
Comp Mole Frac (HCl)		---	---	---	---	---
Comp Mole Frac (Helium)		---	---	---	---	---
Comp Mole Frac (CuO.CuCl2*)		---	---	---	---	---
Comp Mole Frac (CuCl2*)		---	---	---	---	---
Comp Mole Frac (H2O)		---	---	---	---	---
Comp Mole Frac (Hydrogen)		---	---	---	---	---
Comp Mole Frac (Oxygen)		---	---	---	---	---
Comp Mole Frac (Nitrogen)		---	---	---	---	---

Name		Qdryer	Qe-needed	QR2	QR3	Qth
Vapour Fraction		---	---	---	---	---
Temperature	(C)	---	---	---	---	---
Pressure	(kPa)	---	---	---	---	---
Molar Flow	(kgmole/h)	---	---	---	---	---
Mass Flow	(kg/h)	---	---	---	---	---
Std Ideal Liq Vol Flow	(m3/h)	---	---	---	---	---
Heat Flow	(MW)	269.806739	178.050000 *	37.4460802	89.2330737	350.005241
Molar Enthalpy	(kJ/kgmole)	---	---	---	---	---
Comp Mass Frac (CuCl*)		---	---	---	---	---
Comp Mass Frac (HCl)		---	---	---	---	---
Comp Mass Frac (Helium)		---	---	---	---	---
Comp Mass Frac (CuO.CuCl2*)		---	---	---	---	---
Comp Mass Frac (CuCl2*)		---	---	---	---	---
Comp Mass Frac (H2O)		---	---	---	---	---
Comp Mass Frac (Hydrogen)		---	---	---	---	---
Comp Mass Frac (Oxygen)		---	---	---	---	---
Comp Mass Frac (Nitrogen)		---	---	---	---	---
Comp Mole Frac (CuCl*)		---	---	---	---	---
Comp Mole Frac (HCl)		---	---	---	---	---
Comp Mole Frac (Helium)		---	---	---	---	---
Comp Mole Frac (CuO.CuCl2*)		---	---	---	---	---
Comp Mole Frac (CuCl2*)		---	---	---	---	---
Comp Mole Frac (H2O)		---	---	---	---	---
Comp Mole Frac (Hydrogen)		---	---	---	---	---
Comp Mole Frac (Oxygen)		---	---	---	---	---
Comp Mole Frac (Nitrogen)		---	---	---	---	---

Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc Level
CRV-101	Conversion Reactor	10- H2O	11 - CuOCuCl2	No	500.0 *

* Specified by user.

Unit Ops (continued)

Operation Name	Operation Type	Feeds	Products	Ignored	Calc Level
CRV-101	Conversion Reactor	6- CuCl2 hot	22- HCl + H2O	No	500.0 *
		33- Hot Extra Water	QR2		
		QR2			
CRV-102	Conversion Reactor	12 - CuOCuCl2	15- CuCl.l	No	500.0 *
		QR3	13- Oxygen		
			QR3		
CRV-100	Conversion Reactor	1.2	4- CuCl2	No	500.0 *
		2- CuCl	3-H2		
		Q NA	Q NA		
E-105	Cooler	41- He	42- He	No	500.0 *
			QR3		
E-108	Cooler	42- He	43- He	No	500.0 *
			QR2		
E-109	Cooler	43- He	44- He	No	500.0 *
			Q CuCl2 heat		
E-110	Cooler	46- He	47- He	No	500.0 *
			Qe-needed		
E-116	Cooler	51 He side	52- He side	No	500.0 *
			Qth		
E-101	Cooler	24	24.1	No	500.0 *
			Q NA2		
E-113	Cooler	44- He	45- He	No	500.0 *
			Q extra heat		
E-106	Heater	5- CuCl2 dry	6- CuCl2 hot	No	500.0 *
		Q CuCl2 heat			
E-112	Heater	32	33- Hot Extra Water	No	500.0 *
		Q extra heat			
V-100	Tank	4- CuCl2	5- CuCl2 dry	No	500.0 *
		Qdryer	7- H2O Vap		
			Qdryer		
E-117	Heat Exchanger	8.2	9- H2O Cold 0	No	500.0 *
		13- Oxygen	14- O2 cool		
E-104	Heat Exchanger	15- CuCl.l	16- CuCl cooled	No	500.0 *
		17- Air	18- Air		
E-103	Heat Exchanger	11 - CuOCuCl2	12 - CuOCuCl2	No	500.0 *
		18- Air	19- Air		
E-100	Heat Exchanger	9- H2O Cold 0	10- H2O	No	500.0 *
		19- Air	20- Air		
E-107	Heat Exchanger	31	32	No	500.0 *
		22- HCl + H2O	23		
E-102	Heat Exchanger	27	28	No	500.0 *
		20- Air	21		
E-111	Heat Exchanger	29	30	No	500.0 *
		23	24		
MIX-101	Mixer	45- He	48-He out	No	500.0 *
		47- He			
MIX-102	Mixer	28	31	No	500.0 *
		30			
MIX-103	Mixer	8- H2O Cold	8.2	No	500.0 *
		8.1			
MIX-104	Mixer	1- HCl	1.2	No	500.0 *
		1.1 Equavalent water			
TEE-100	Tee	50 - He big	40 - Helium	No	500.0 *
			51 He side		
TEE-101	Tee	40 - Helium	41- He	No	500.0 *
			46- He		
TEE-102	Tee	26- Extra water	27	No	500.0 *

Unit Ops (continued)

Operation Name	Operation Type	Feeds	Products	Ignored	Calc Level
TEE-102	Tee		29	No	500.0 *
SET-1	Set			No	500.0 *
SET-2	Set			No	500.0 *
SET-3	Set			No	500.0 *
SET-4	Set			No	500.0 *
SET-5	Set			No	500.0 *
SET-6	Set			No	500.0 *
P-100	Pump	24.1 Q pump	25	No	500.0 *

Table A-5: Mass and Energy Balance for the Kemp Model with extra steam purchased

Streams

Fluid Pkg: All

Name		1- HCl	1.1 H2O extra	2- CuCl	3-H2	4- CuCl2
Vapour Fraction		0.6756	0.0000	0.0000	1.0000	0.0000
Temperature	(C)	70.00 *	70.00 *	70.00 *	70.00	70.00 *
Pressure	(kPa)	2400 *	2400 *	2400 *	2400	2400
Molar Flow	(kgmole/h)	6500.0	21666	4333.3	2195.6	28137
Mass Flow	(kg/h)	197030	390312	428991	4919.96	1.01142e+006
Std Ideal Liq Vol Flow	(m3/h)	220.6	391.1	103.6	63.03	601.1
Heat Flow	(MW)	-279.893499	-1701.24728	-159.858126	-1.29013024	-2112.35668
Molar Enthalpy	(kJ/kgmole)	-1.550e+005	-2.827e+005	-1.328e+005	-2115	-2.703e+005
Comp Mass Frac (CuCl*)		0.0000 *	0.0000 *	1.0000 *	0.0000	0.0000
Comp Mass Frac (HCl)		0.8019 *	0.0000 *	0.0000 *	0.0001	0.0000
Comp Mass Frac (Helium)		0.0000 *	0.0000 *	0.0000 *	0.0000	0.0000
Comp Mass Frac (CuO.CuCl2*)		0.0000 *	0.0000 *	0.0000 *	0.0000	0.0000
Comp Mass Frac (CuCl2*)		0.0000 *	0.0000 *	0.0000 *	0.0000	0.5760
Comp Mass Frac (H2O)		0.1981 *	1.0000 *	0.0000 *	0.1129	0.4239
Comp Mass Frac (Hydrogen)		0.0000 *	0.0000 *	0.0000 *	0.8870	0.0000
Comp Mass Frac (Oxygen)		0.0000 *	0.0000 *	0.0000 *	0.0000	0.0000
Comp Mass Frac (Nitrogen)		0.0000 *	0.0000 *	0.0000 *	0.0000	0.0000
Comp Mole Frac (CuCl*)		0.0000 *	0.0000 *	1.0000 *	0.0000	0.0000
Comp Mole Frac (HCl)		0.6667 *	0.0000 *	0.0000 *	0.0000	0.0000
Comp Mole Frac (Helium)		0.0000 *	0.0000 *	0.0000 *	0.0000	0.0000
Comp Mole Frac (CuO.CuCl2*)		0.0000 *	0.0000 *	0.0000 *	0.0000	0.0000
Comp Mole Frac (CuCl2*)		0.0000 *	0.0000 *	0.0000 *	0.0000	0.1540
Comp Mole Frac (H2O)		0.3333 *	1.0000 *	0.0000 *	0.0140	0.8459
Comp Mole Frac (Hydrogen)		0.0000 *	0.0000 *	0.0000 *	0.9859	0.0001
Comp Mole Frac (Oxygen)		0.0000 *	0.0000 *	0.0000 *	0.0000	0.0000
Comp Mole Frac (Nitrogen)		0.0000 *	0.0000 *	0.0000 *	0.0000	0.0000

Name		5- CuCl2 dry	5.1- CuCl2 dry	6- CuCl2 hot	7- H2O Vap	8 Water
Vapour Fraction		0.0000	0.0000	0.0000	1.0000	0.0000
Temperature	(C)	82.00	110.6	370.0 *	82.00 *	25.00 *
Pressure	(kPa)	50.00 *	50.00	50.00	50.00 *	101.3 *
Molar Flow	(kgmole/h)	4333.3	4333.3	4333.3	23804	13000 *
Mass Flow	(kg/h)	582624	582624	582624	428793	234196
Std Ideal Liq Vol Flow	(m3/h)	171.4	171.4	171.4	429.7	234.7
Heat Flow	(MW)	-242.247002	-239.465869	-214.281041	-1586.29185	-1033.57463
Molar Enthalpy	(kJ/kgmole)	-2.013e+005	-1.989e+005	-1.780e+005	-2.399e+005	-2.862e+005
Comp Mass Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (Helium)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (CuCl2*)		1.0000	1.0000	1.0000	0.0000	0.0000 *
Comp Mass Frac (H2O)		0.0000	0.0000	0.0000	1.0000	1.0000 *
Comp Mass Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (Helium)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (CuCl2*)		1.0000	1.0000	1.0000	0.0000	0.0000 *
Comp Mole Frac (H2O)		0.0000	0.0000	0.0000	0.9999	1.0000 *
Comp Mole Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0001	0.0000 *
Comp Mole Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000 *

* Specified by user.

Streams (continued)

Fluid Pkg: All

Name	9	10- H2O	11- Steam bought	12- CuOCuCl2	13- CuOCuCl2 2
Vapour Fraction	1.0000	1.0000	1.0000	0.0000	0.0000
Temperature (C)	220.0 *	400.0 *	400.0 *	370.0 *	388.0 *
Pressure (kPa)	50.00 *	50.00 *	50.00 *	50.00	101.3 *
Molar Flow (kgmole/h)	13000	13000	13000	2166.7	2166.7
Mass Flow (kg/h)	234196	234196	234196	463659	463659
Std Ideal Liq Vol Flow (m3/h)	234.7	234.7	234.7	113.6	113.6
Heat Flow (MW)	-849.129767	-825.504554	-825.504554	-205.698967	-204.261365
Molar Enthalpy (kJ/kgmole)	-2.351e+005	-2.286e+005	-2.286e+005	-3.418e+005	-3.394e+005
Comp Mass Frac (CuCl*)	0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mass Frac (HCl)	0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mass Frac (Helium)	0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mass Frac (CuO.CuCl2*)	0.0000	0.0000	0.0000 *	1.0000	1.0000
Comp Mass Frac (CuCl2*)	0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mass Frac (H2O)	1.0000	1.0000	1.0000 *	0.0000	0.0000
Comp Mass Frac (Hydrogen)	0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mass Frac (Oxygen)	0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mass Frac (Nitrogen)	0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mole Frac (CuCl*)	0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mole Frac (HCl)	0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mole Frac (Helium)	0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mole Frac (CuO.CuCl2*)	0.0000	0.0000	0.0000 *	1.0000	1.0000
Comp Mole Frac (CuCl2*)	0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mole Frac (H2O)	1.0000	1.0000	1.0000 *	0.0000	0.0000
Comp Mole Frac (Hydrogen)	0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mole Frac (Oxygen)	0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mole Frac (Nitrogen)	0.0000	0.0000	0.0000 *	0.0000	0.0000

Name	14- CuOCuCl2 3	15- Oxygen	16- O2 cool	17 - O2 cool	18- CuCl-l
Vapour Fraction	0.0000	1.0000	1.0000	1.0000	0.0000
Temperature (C)	430.0 *	530.0 *	385.8	90.00 *	530.0
Pressure (kPa)	101.3	101.3	101.3	101.3	101.3
Molar Flow (kgmole/h)	2166.7	1083.3	1083.3	1083.3	4333.3
Mass Flow (kg/h)	463659	34666.6	34666.6	34666.6	428995
Std Ideal Liq Vol Flow (m3/h)	113.6	30.47	30.47	30.47	103.6
Heat Flow (MW)	-200.877880	4.79366584	3.35606371	0.574930699	-110.525011
Molar Enthalpy (kJ/kgmole)	-3.338e+005	1.593e+004	1.115e+004	1911	-9.182e+004
Comp Mass Frac (CuCl*)	0.0000	0.0000	0.0000	0.0000	1.0000
Comp Mass Frac (HCl)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Helium)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuO.CuCl2*)	1.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuCl2*)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (H2O)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Hydrogen)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Oxygen)	0.0000	1.0000	1.0000	1.0000	0.0000
Comp Mass Frac (Nitrogen)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl*)	0.0000	0.0000	0.0000	0.0000	1.0000
Comp Mole Frac (HCl)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Helium)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuO.CuCl2*)	1.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl2*)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (H2O)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Hydrogen)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Oxygen)	0.0000	1.0000	1.0000	1.0000	0.0000
Comp Mole Frac (Nitrogen)	0.0000	0.0000	0.0000	0.0000	0.0000

Streams (continued)

Fluid Pkg: All

Name		19- CuCl cooled	20- HCl + H2O	21- Recycle	22- Recycle	23- HCl + H2O recycle
Vapour Fraction		0.0000	1.0000	0.6329	0.0000 *	---
Temperature	(C)	70.00 *	370.0	74.56	-95.85	---
Pressure	(kPa)	2400 *	50.00	50.00	50.00	2400 *
Molar Flow	(kgmole/h)	4333.3	28167	28167	28167	28167
Mass Flow	(kg/h)	428995	587356	587356	587356	587356
Std Ideal Liq Vol Flow	(m3/h)	103.6	611.8	611.8	611.8	611.8
Heat Flow	(MW)	-159.859418	-1619.65859	-1820.66505	-2314.15998	-2313.75582
Molar Enthalpy	(kJ/kgmole)	-1.328e+005	-2.070e+005	-2.327e+005	-2.958e+005	-2.957e+005
Comp Mass Frac (CuCl*)		1.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (HCl)		0.0000	0.2690	0.2690	0.2690	0.2690
Comp Mass Frac (Helium)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (H2O)		0.0000	0.7310	0.7310	0.7310	0.7310
Comp Mass Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl*)		1.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (HCl)		0.0000	0.1538	0.1538	0.1538	0.1538
Comp Mole Frac (Helium)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (H2O)		0.0000	0.8462	0.8462	0.8462	0.8462
Comp Mole Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000

Name		24- Air	25- Air	26- Air	27- Air	28- Air
Vapour Fraction		1.0000	1.0000	1.0000	1.0000	1.0000
Temperature	(C)	25.00 *	225.0 *	25.00 *	490.0 *	459.3
Pressure	(kPa)	200.0 *	200.0	200.0 *	200.0	200.0
Molar Flow	(kgmole/h)	1.2133e+005	1.2133e+005	12493	12493	12493
Mass Flow	(kg/h)	3.49024e+006	3.49024e+006	359363	359363	359363
Std Ideal Liq Vol Flow	(m3/h)	4064	4064	418.4	418.4	418.4
Heat Flow	(MW)	-0.540953135	200.465513	-5.56978373e-002	49.2787095	45.8952245
Molar Enthalpy	(kJ/kgmole)	-16.05	5948	-16.05	1.420e+004	1.323e+004
Comp Mass Frac (CuCl*)		0.0000 *	0.0000	0.0000 *	0.0000	0.0000
Comp Mass Frac (HCl)		0.0000 *	0.0000	0.0000 *	0.0000	0.0000
Comp Mass Frac (Helium)		0.0000 *	0.0000	0.0000 *	0.0000	0.0000
Comp Mass Frac (CuO.CuCl2*)		0.0000 *	0.0000	0.0000 *	0.0000	0.0000
Comp Mass Frac (CuCl2*)		0.0000 *	0.0000	0.0000 *	0.0000	0.0000
Comp Mass Frac (H2O)		0.0000 *	0.0000	0.0000 *	0.0000	0.0000
Comp Mass Frac (Hydrogen)		0.0000 *	0.0000	0.0000 *	0.0000	0.0000
Comp Mass Frac (Oxygen)		0.2100 *	0.2100	0.2100 *	0.2100	0.2100
Comp Mass Frac (Nitrogen)		0.7900 *	0.7900	0.7900 *	0.7900	0.7900
Comp Mole Frac (CuCl*)		0.0000 *	0.0000	0.0000 *	0.0000	0.0000
Comp Mole Frac (HCl)		0.0000 *	0.0000	0.0000 *	0.0000	0.0000
Comp Mole Frac (Helium)		0.0000 *	0.0000	0.0000 *	0.0000	0.0000
Comp Mole Frac (CuO.CuCl2*)		0.0000 *	0.0000	0.0000 *	0.0000	0.0000
Comp Mole Frac (CuCl2*)		0.0000 *	0.0000	0.0000 *	0.0000	0.0000
Comp Mole Frac (H2O)		0.0000 *	0.0000	0.0000 *	0.0000	0.0000
Comp Mole Frac (Hydrogen)		0.0000 *	0.0000	0.0000 *	0.0000	0.0000
Comp Mole Frac (Oxygen)		0.1888 *	0.1888	0.1888 *	0.1888	0.1888
Comp Mole Frac (Nitrogen)		0.8112 *	0.8112	0.8112 *	0.8112	0.8112

* Specified by user.

Streams (continued)

Fluid Pkg: All

Name		29- Air	30- Air	31- Air	40- He in	41- He
Vapour Fraction		1.0000	1.0000	1.0000	1.0000	1.0000
Temperature	(C)	240.4	226.4	60.64	720.8 *	606.4
Pressure	(kPa)	200.0	200.0	200.0	3000 *	3000
Molar Flow	(kgmole/h)	12493	1.3383e+005	1.3383e+005	1.4389e+005	1.4389e+005
Mass Flow	(kg/h)	359363	3.84960e+006	3.84960e+006	576000	576000
Std Ideal Liq Vol Flow	(m3/h)	418.4	4482	4482	4643	4643
Heat Flow	(MW)	22.2700113	222.735524	38.2906631	578.639862	483.493327
Molar Enthalpy	(kJ/kgmole)	6417	5992	1030	1.448e+004	1.210e+004
Comp Mass Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (HCl)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (Helium)		0.0000	0.0000	0.0000	1.0000 *	1.0000
Comp Mass Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (H2O)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (Oxygen)		0.2100	0.2100	0.2100	0.0000 *	0.0000
Comp Mass Frac (Nitrogen)		0.7900	0.7900	0.7900	0.0000 *	0.0000
Comp Mole Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (HCl)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (Helium)		0.0000	0.0000	0.0000	1.0000 *	1.0000
Comp Mole Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (H2O)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (Oxygen)		0.1888	0.1888	0.1888	0.0000 *	0.0000
Comp Mole Frac (Nitrogen)		0.8112	0.8112	0.8112	0.0000 *	0.0000

Name		42- He	43- He	44- He Out	50	51
Vapour Fraction		1.0000	1.0000	1.0000	1.0000	1.0000
Temperature	(C)	558.4	528.1	300.0	720.8	720.8
Pressure	(kPa)	3000	3000	3000	3000	3000
Molar Flow	(kgmole/h)	1.4389e+005	1.4389e+005	1.4389e+005	2.8779e+005	1.4389e+005
Mass Flow	(kg/h)	576000	576000	576000 *	1.15200e+006	576000
Std Ideal Liq Vol Flow	(m3/h)	4643	4643	4643	9286	4643
Heat Flow	(MW)	443.560730	418.375902	228.663603	1157.27972	578.639862
Molar Enthalpy	(kJ/kgmole)	1.110e+004	1.047e+004	5721	1.448e+004	1.448e+004
Comp Mass Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Helium)		1.0000	1.0000	1.0000	1.0000	1.0000
Comp Mass Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (H2O)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Helium)		1.0000	1.0000	1.0000	1.0000	1.0000
Comp Mole Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (H2O)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000

* Specified by user.

Streams (continued)

Fluid Pkg: All

Name		52	Q CuCl2 heat	Q pump	Qdryer	Qe-needed
Vapour Fraction		1.0000	---	---	---	---
Temperature	(C)	300.0	---	---	---	---
Pressure	(kPa)	3000	---	---	---	---
Molar Flow	(kgmole/h)	1.4389e+005	---	---	---	---
Mass Flow	(kg/h)	576000	---	---	---	---
Std Ideal Liq Vol Flow	(m3/h)	4643	---	---	---	---
Heat Flow	(MW)	228.663603	25.1848285	0.404167658	283.817833	189.712298 *
Molar Enthalpy	(kJ/kgmole)	5721	---	---	---	---
Comp Mass Frac (CuCl*)		0.0000	---	---	---	---
Comp Mass Frac (HCl)		0.0000	---	---	---	---
Comp Mass Frac (Helium)		1.0000	---	---	---	---
Comp Mass Frac (CuO.CuCl2*)		0.0000	---	---	---	---
Comp Mass Frac (CuCl2*)		0.0000	---	---	---	---
Comp Mass Frac (H2O)		0.0000	---	---	---	---
Comp Mass Frac (Hydrogen)		0.0000	---	---	---	---
Comp Mass Frac (Oxygen)		0.0000	---	---	---	---
Comp Mass Frac (Nitrogen)		0.0000	---	---	---	---
Comp Mole Frac (CuCl*)		0.0000	---	---	---	---
Comp Mole Frac (HCl)		0.0000	---	---	---	---
Comp Mole Frac (Helium)		1.0000	---	---	---	---
Comp Mole Frac (CuO.CuCl2*)		0.0000	---	---	---	---
Comp Mole Frac (CuCl2*)		0.0000	---	---	---	---
Comp Mole Frac (H2O)		0.0000	---	---	---	---
Comp Mole Frac (Hydrogen)		0.0000	---	---	---	---
Comp Mole Frac (Oxygen)		0.0000	---	---	---	---
Comp Mole Frac (Nitrogen)		0.0000	---	---	---	---

Name		QNA1	QNA2	QR2	QR3	Qth
Vapour Fraction		---	---	---	---	---
Temperature	(C)	---	---	---	---	---
Pressure	(kPa)	---	---	---	---	---
Molar Flow	(kgmole/h)	---	---	---	---	---
Mass Flow	(kg/h)	---	---	---	---	---
Std Ideal Liq Vol Flow	(m3/h)	---	---	---	---	---
Heat Flow	(MW)	27.3520638	493.494932	39.9325967	95.1465348	349.976258
Molar Enthalpy	(kJ/kgmole)	---	---	---	---	---
Comp Mass Frac (CuCl*)		---	---	---	---	---
Comp Mass Frac (HCl)		---	---	---	---	---
Comp Mass Frac (Helium)		---	---	---	---	---
Comp Mass Frac (CuO.CuCl2*)		---	---	---	---	---
Comp Mass Frac (CuCl2*)		---	---	---	---	---
Comp Mass Frac (H2O)		---	---	---	---	---
Comp Mass Frac (Hydrogen)		---	---	---	---	---
Comp Mass Frac (Oxygen)		---	---	---	---	---
Comp Mass Frac (Nitrogen)		---	---	---	---	---
Comp Mole Frac (CuCl*)		---	---	---	---	---
Comp Mole Frac (HCl)		---	---	---	---	---
Comp Mole Frac (Helium)		---	---	---	---	---
Comp Mole Frac (CuO.CuCl2*)		---	---	---	---	---
Comp Mole Frac (CuCl2*)		---	---	---	---	---
Comp Mole Frac (H2O)		---	---	---	---	---
Comp Mole Frac (Hydrogen)		---	---	---	---	---
Comp Mole Frac (Oxygen)		---	---	---	---	---
Comp Mole Frac (Nitrogen)		---	---	---	---	---

Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc Level
CRV-101	Conversion Reactor	10- H2O	12- CuOCuCl2	No	500.0 *

Unit Ops (continued)

Operation Name	Operation Type	Feeds	Products	Ignored	Calc Level
CRV-101	Conversion Reactor	6- CuCl2 hot 11- Steam bought QR2	20- HCl + H2O QR2	No	500.0 *
CRV-102	Conversion Reactor	14- CuOCuCl2 3 QR3	18- CuCl-l 15- Oxygen QR3	No	500.0 *
CRV-100	Conversion Reactor	1- HCl 2- CuCl 1.1 H2O extra QNA1	4- CuCl2 3-H2 QNA1	No	500.0 *
E-105	Cooler	40- He in	41- He QR3	No	500.0 *
E-108	Cooler	42- He	43- He Q CuCl2 heat	No	500.0 *
E-109	Cooler	43- He	44- He Out Qe-needed	No	500.0 *
E-112	Cooler	41- He	42- He QR2	No	500.0 *
E-111	Cooler	51	52 Qth	No	500.0 *
E-107	Cooler	21- Recycle	22- Recycle QNA2	No	500.0 *
E-106	Heater	5.1- CuCl2 dry Q CuCl2 heat	6- CuCl2 hot	No	500.0 *
V-100	Tank	4- CuCl2 Qdryer	5- CuCl2 dry 7- H2O Vap Qdryer	No	500.0 *
E-101	Heat Exchanger	12- CuOCuCl2 15- Oxygen	13- CuOCuCl2 2 16- O2 cool	No	500.0 *
E-104	Heat Exchanger	18- CuCl-l 26- Air	19- CuCl cooled 27- Air	No	500.0 *
E-103	Heat Exchanger	13- CuOCuCl2 2 27- Air	14- CuOCuCl2 3 28- Air	No	500.0 *
E-100	Heat Exchanger	9 28- Air	10- H2O 29- Air	No	500.0 *
E-110	Heat Exchanger	20- HCl + H2O 24- Air	21- Recycle 25- Air	No	500.0 *
E-114	Heat Exchanger	30- Air 8 Water	31- Air 9	No	500.0 *
E-115	Heat Exchanger	5- CuCl2 dry 16- O2 cool	5.1- CuCl2 dry 17 - O2 cool	No	500.0 *
MIX-101	Mixer	25- Air 29- Air	30- Air	No	500.0 *
TEE-100	Tee	50	40- He in 51	No	500.0 *
SET-1	Set			No	500.0 *
SET-2	Set			No	500.0 *
SET-3	Set			No	500.0 *
SET-4	Set			No	500.0 *
SET-5	Set			No	500.0 *
SET-6	Set			No	500.0 *
P-100	Pump	22- Recycle Q pump	23- HCl + H2O recycle	No	500.0 *

* Specified by user.

Table A-6: Mass and Energy Balance for the Kemp Model with electricity purchased

Streams

Fluid Pkg: All

Name	1- HCl	2- CuCl	3-H2	4- CuCl2	5- CuCl2 dry
Vapour Fraction	0.6756	0.0000	1.0000	0.0000	0.0000
Temperature (C)	70.00 *	70.00 *	70.00	70.00 *	82.00
Pressure (kPa)	2400 *	2400 *	2400	2400	50.00 *
Molar Flow (kgmole/h)	7095.0	4730.0	2398.5	7061.5	4730.0
Mass Flow (kg/h)	215065	468265	5374.46	677961	635962
Std Ideal Liq Vol Flow (m3/h)	240.8	113.1	68.85	229.1	187.0
Heat Flow (MW)	-305.514520	-174.493038	-1.40916828	-448.753879	-264.423826
Molar Enthalpy (kJ/kgmole)	-1.550e+005	-1.328e+005	-2115	-2.288e+005	-2.013e+005
Comp Mass Frac (CuCl*)	0.0000 *	1.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (HCl)	0.8019 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (Helium)	0.0000 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (CuO.CuCl2*)	0.0000 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (CuCl2*)	0.0000 *	0.0000 *	0.0000	0.9380	1.0000
Comp Mass Frac (H2O)	0.1981 *	0.0000 *	0.1129	0.0619	0.0000
Comp Mass Frac (Hydrogen)	0.0000 *	0.0000 *	0.8871	0.0000	0.0000
Comp Mass Frac (Oxygen)	0.0000 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (Nitrogen)	0.0000 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl*)	0.0000 *	1.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (HCl)	0.6667 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (Helium)	0.0000 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (CuO.CuCl2*)	0.0000 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl2*)	0.0000 *	0.0000 *	0.0000	0.6698	1.0000
Comp Mole Frac (H2O)	0.3333 *	0.0000 *	0.0140	0.3301	0.0000
Comp Mole Frac (Hydrogen)	0.0000 *	0.0000 *	0.9860	0.0000	0.0000
Comp Mole Frac (Oxygen)	0.0000 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (Nitrogen)	0.0000 *	0.0000 *	0.0000	0.0000	0.0000

Name	5.1- CuCl2 dry	6- CuCl2 hot	7- H2O Vap	8- Extra Water	9
Vapour Fraction	0.0000	0.0000	1.0000	0.0000	1.0000
Temperature (C)	110.6	370.0 *	82.00 *	25.00 *	250.0 *
Pressure (kPa)	50.00	50.00	50.00 *	101.3 *	50.00 *
Molar Flow (kgmole/h)	4730.0	4730.0	2331.5	4730.0 *	4730.0
Mass Flow (kg/h)	635962	635962	41999.1	85211.4	85211.4
Std Ideal Liq Vol Flow (m3/h)	187.0	187.0	42.09	85.38	85.38
Heat Flow (MW)	-261.388124	-233.897573	-155.373058	-376.062153	-307.554038
Molar Enthalpy (kJ/kgmole)	-1.989e+005	-1.780e+005	-2.399e+005	-2.862e+005	-2.341e+005
Comp Mass Frac (CuCl*)	0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (HCl)	0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (Helium)	0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (CuO.CuCl2*)	0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (CuCl2*)	1.0000	1.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (H2O)	0.0000	0.0000	1.0000	1.0000 *	1.0000
Comp Mass Frac (Hydrogen)	0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (Oxygen)	0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (Nitrogen)	0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (CuCl*)	0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (HCl)	0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (Helium)	0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (CuO.CuCl2*)	0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (CuCl2*)	1.0000	1.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (H2O)	0.0000	0.0000	0.9999	1.0000 *	1.0000
Comp Mole Frac (Hydrogen)	0.0000	0.0000	0.0001	0.0000 *	0.0000
Comp Mole Frac (Oxygen)	0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (Nitrogen)	0.0000	0.0000	0.0000	0.0000 *	0.0000

* Specified by user.

Streams (continued)

Fluid Pkg: All

Name		10- H2O	11- CuCl2	12- CuOCuCl2	13- CuOCuCl2	14- Oxygen
Vapour Fraction		1.0000	0.0000	0.0000	0.0000	1.0000
Temperature	(C)	400.0 *	370.0 *	388.0 *	430.0 *	530.0 *
Pressure	(kPa)	50.00 *	50.00	101.3 *	101.3	101.3
Molar Flow	(kgmole/h)	4730.0	2365.0	2365.0	2365.0	1182.5
Mass Flow	(kg/h)	85211.4	506107	506107	506107	37840.0
Std Ideal Liq Vol Flow	(m3/h)	85.38	124.0	124.0	124.0	33.26
Heat Flow	(MW)	-300.356657	-224.529891	-222.960673	-219.267422	5.23248068
Molar Enthalpy	(kJ/kgmole)	-2.286e+005	-3.418e+005	-3.394e+005	-3.338e+005	1.593e+004
Comp Mass Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Helium)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuO.CuCl2*)		0.0000	1.0000	1.0000	1.0000	0.0000
Comp Mass Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (H2O)		1.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	1.0000
Comp Mass Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Helium)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuO.CuCl2*)		0.0000	1.0000	1.0000	1.0000	0.0000
Comp Mole Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (H2O)		1.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	1.0000
Comp Mole Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000

Name		15- O2 cool	16- O2 cool	17- CuCl-l	18- CuCl cooled	19- HCl + H2O
Vapour Fraction		1.0000	1.0000	0.0000	0.0000	1.0000
Temperature	(C)	385.8	90.00 *	530.0	70.00 *	370.0
Pressure	(kPa)	101.3	101.3	101.3	2400 *	50.00
Molar Flow	(kgmole/h)	1182.5	1182.5	4730.0	4730.0	7095.0
Mass Flow	(kg/h)	37840.0	37840.0	468269	468269	215065
Std Ideal Liq Vol Flow	(m3/h)	33.26	33.26	113.1	113.1	240.8
Heat Flow	(MW)	3.66326261	0.627560174	-120.643507	-174.494448	-258.798069
Molar Enthalpy	(kJ/kgmole)	1.115e+004	1911	-9.182e+004	-1.328e+005	-1.313e+005
Comp Mass Frac (CuCl*)		0.0000	0.0000	1.0000	1.0000	0.0000
Comp Mass Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.8019
Comp Mass Frac (Helium)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (H2O)		0.0000	0.0000	0.0000	0.0000	0.1981
Comp Mass Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Oxygen)		1.0000	1.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl*)		0.0000	0.0000	1.0000	1.0000	0.0000
Comp Mole Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.6667
Comp Mole Frac (Helium)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (H2O)		0.0000	0.0000	0.0000	0.0000	0.3333
Comp Mole Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Oxygen)		1.0000	1.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000

Streams (continued)

Fluid Pkg: All

Name		20- Recycle	21	22- Liquid HCl + H2O	23	24- Air
Vapour Fraction		0.7834	1.0000	0.0000 *	0.0000	1.0000
Temperature	(C)	40.30	70.00 *	-95.85	-95.37	25.00 *
Pressure	(kPa)	50.00	50.00	50.00	2400 *	200.0 *
Molar Flow	(kgmole/h)	7095.0	7095.0	7095.0	7095.0	23650
Mass Flow	(kg/h)	215065	215065	215065	215065	680301
Std Ideal Liq Vol Flow	(m3/h)	240.8	240.8	240.8	240.8	792.1
Heat Flow	(MW)	-297.977307	-277.510594	-342.682214	-342.525243	-0.105440050
Molar Enthalpy	(kJ/kgmole)	-1.512e+005	-1.408e+005	-1.739e+005	-1.738e+005	-16.05
Comp Mass Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (HCl)		0.8019	0.8019	0.8019	0.8019	0.0000 *
Comp Mass Frac (Helium)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (H2O)		0.1981	0.1981	0.1981	0.1981	0.0000 *
Comp Mass Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	0.2100 *
Comp Mass Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.7900 *
Comp Mole Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (HCl)		0.6667	0.6667	0.6667	0.6667	0.0000 *
Comp Mole Frac (Helium)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (H2O)		0.3333	0.3333	0.3333	0.3333	0.0000 *
Comp Mole Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	0.1888 *
Comp Mole Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.8112 *

Name		25- Air	26- Air	27- Air	28- Air	29- Air
Vapour Fraction		1.0000	1.0000	1.0000	1.0000	1.0000
Temperature	(C)	225.0 *	25.00 *	490.0 *	459.3	399.1
Pressure	(kPa)	200.0	200.0 *	200.0	200.0	200.0
Molar Flow	(kgmole/h)	23650	13637	13637	13637	13637
Mass Flow	(kg/h)	680301	392263	392263	392263	392263
Std Ideal Liq Vol Flow	(m3/h)	792.1	456.7	456.7	456.7	456.7
Heat Flow	(MW)	39.0737983	-6.07969396e-002	53.7901446	50.0968939	42.8995132
Molar Enthalpy	(kJ/kgmole)	5948	-16.05	1.420e+004	1.323e+004	1.133e+004
Comp Mass Frac (CuCl*)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (HCl)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (Helium)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (CuO.CuCl2*)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (CuCl2*)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (H2O)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (Hydrogen)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (Oxygen)		0.2100	0.2100 *	0.2100	0.2100	0.2100
Comp Mass Frac (Nitrogen)		0.7900	0.7900 *	0.7900	0.7900	0.7900
Comp Mole Frac (CuCl*)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (HCl)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (Helium)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (CuO.CuCl2*)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl2*)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (H2O)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (Hydrogen)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (Oxygen)		0.1888	0.1888 *	0.1888	0.1888	0.1888
Comp Mole Frac (Nitrogen)		0.8112	0.8112 *	0.8112	0.8112	0.8112

Streams (continued)

Fluid Pkg: All

Name		30- Air	31- Air	40- He In	41- He	42- He
Vapour Fraction		1.0000	1.0000	1.0000	1.0000	1.0000
Temperature	(C)	289.3	69.80	720.8 *	720.8	512.7
Pressure	(kPa)	200.0	200.0	3000 *	3000	3000
Molar Flow	(kgmole/h)	37286	37286	1.4389e+005	86336	86336
Mass Flow	(kg/h)	1.07256e+006	1.07256e+006	576000 *	345600	345600
Std Ideal Liq Vol Flow	(m3/h)	1249	1249	4643	2786	2786
Heat Flow	(MW)	81.9733115	13.4651960	578.639862	347.183917	243.327521
Molar Enthalpy	(kJ/kgmole)	7915	1300	1.448e+004	1.448e+004	1.015e+004
Comp Mass Frac (CuCl*)		0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mass Frac (HCl)		0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mass Frac (Helium)		0.0000	0.0000	1.0000 *	1.0000	1.0000
Comp Mass Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mass Frac (CuCl2*)		0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mass Frac (H2O)		0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mass Frac (Hydrogen)		0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mass Frac (Oxygen)		0.2100	0.2100	0.0000 *	0.0000	0.0000
Comp Mass Frac (Nitrogen)		0.7900	0.7900	0.0000 *	0.0000	0.0000
Comp Mole Frac (CuCl*)		0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mole Frac (HCl)		0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mole Frac (Helium)		0.0000	0.0000	1.0000 *	1.0000	1.0000
Comp Mole Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mole Frac (CuCl2*)		0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mole Frac (H2O)		0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mole Frac (Hydrogen)		0.0000	0.0000	0.0000 *	0.0000	0.0000
Comp Mole Frac (Oxygen)		0.1888	0.1888	0.0000 *	0.0000	0.0000
Comp Mole Frac (Nitrogen)		0.8112	0.8112	0.0000 *	0.0000	0.0000

Name		43- He	44- He	45- He for electricity	46- He	47- He Out
Vapour Fraction		1.0000	1.0000	1.0000	1.0000	1.0000
Temperature	(C)	410.6	355.6	720.8	216.8	300.1
Pressure	(kPa)	3000	3000	3000	3000	3000
Molar Flow	(kgmole/h)	86336	86336	57557	57557	1.4389e+005
Mass Flow	(kg/h)	345600	345600	230400	230400	576000
Std Ideal Liq Vol Flow	(m3/h)	2786	2786	1857	1857	4643
Heat Flow	(MW)	192.401251	164.910700	231.455945	63.7660519	228.676752
Molar Enthalpy	(kJ/kgmole)	8023	6876	1.448e+004	3988	5721
Comp Mass Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Helium)		1.0000	1.0000	1.0000	1.0000	1.0000
Comp Mass Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (H2O)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Helium)		1.0000	1.0000	1.0000	1.0000	1.0000
Comp Mole Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (H2O)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000

Streams (continued)

Fluid Pkg: All

Name		50	51	52	Q CuCl2 heat	Q pump
Vapour Fraction		1.0000	1.0000	1.0000	---	---
Temperature	(C)	720.8	720.8	300.1	---	---
Pressure	(kPa)	3000	3000	3000	---	---
Molar Flow	(kgmole/h)	2.8779e+005	1.4389e+005	1.4389e+005	---	---
Mass Flow	(kg/h)	1.15200e+006	576000	576000	---	---
Std Ideal Liq Vol Flow	(m3/h)	9286	4643	4643	---	---
Heat Flow	(MW)	1157.27972	578.639862	228.676752	27.4905512	0.156971256
Molar Enthalpy	(kJ/kgmole)	1.448e+004	1.448e+004	5721	---	---
Comp Mass Frac (CuCl*)		0.0000	0.0000	0.0000	---	---
Comp Mass Frac (HCl)		0.0000	0.0000	0.0000	---	---
Comp Mass Frac (Helium)		1.0000	1.0000	1.0000	---	---
Comp Mass Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	---	---
Comp Mass Frac (CuCl2*)		0.0000	0.0000	0.0000	---	---
Comp Mass Frac (H2O)		0.0000	0.0000	0.0000	---	---
Comp Mass Frac (Hydrogen)		0.0000	0.0000	0.0000	---	---
Comp Mass Frac (Oxygen)		0.0000	0.0000	0.0000	---	---
Comp Mass Frac (Nitrogen)		0.0000	0.0000	0.0000	---	---
Comp Mole Frac (CuCl*)		0.0000	0.0000	0.0000	---	---
Comp Mole Frac (HCl)		0.0000	0.0000	0.0000	---	---
Comp Mole Frac (Helium)		1.0000	1.0000	1.0000	---	---
Comp Mole Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	---	---
Comp Mole Frac (CuCl2*)		0.0000	0.0000	0.0000	---	---
Comp Mole Frac (H2O)		0.0000	0.0000	0.0000	---	---
Comp Mole Frac (Hydrogen)		0.0000	0.0000	0.0000	---	---
Comp Mole Frac (Oxygen)		0.0000	0.0000	0.0000	---	---
Comp Mole Frac (Nitrogen)		0.0000	0.0000	0.0000	---	---

Name		Qdryer	Qe-needed	QNA1	QNA2	QR2
Vapour Fraction		---	---	---	---	---
Temperature	(C)	---	---	---	---	---
Pressure	(kPa)	---	---	---	---	---
Molar Flow	(kgmole/h)	---	---	---	---	---
Mass Flow	(kg/h)	---	---	---	---	---
Std Ideal Liq Vol Flow	(m3/h)	---	---	---	---	---
Heat Flow	(MW)	28.9569947	167.689893 *	29.8445027	65.1716205	50.9262699
Molar Enthalpy	(kJ/kgmole)	---	---	---	---	---
Comp Mass Frac (CuCl*)		---	---	---	---	---
Comp Mass Frac (HCl)		---	---	---	---	---
Comp Mass Frac (Helium)		---	---	---	---	---
Comp Mass Frac (CuO.CuCl2*)		---	---	---	---	---
Comp Mass Frac (CuCl2*)		---	---	---	---	---
Comp Mass Frac (H2O)		---	---	---	---	---
Comp Mass Frac (Hydrogen)		---	---	---	---	---
Comp Mass Frac (Oxygen)		---	---	---	---	---
Comp Mass Frac (Nitrogen)		---	---	---	---	---
Comp Mole Frac (CuCl*)		---	---	---	---	---
Comp Mole Frac (HCl)		---	---	---	---	---
Comp Mole Frac (Helium)		---	---	---	---	---
Comp Mole Frac (CuO.CuCl2*)		---	---	---	---	---
Comp Mole Frac (CuCl2*)		---	---	---	---	---
Comp Mole Frac (H2O)		---	---	---	---	---
Comp Mole Frac (Hydrogen)		---	---	---	---	---
Comp Mole Frac (Oxygen)		---	---	---	---	---
Comp Mole Frac (Nitrogen)		---	---	---	---	---

Streams (continued)

Fluid Pkg: All

Name	QR3	Qth	Qwaste		
Vapour Fraction	---	---	---		
Temperature (C)	---	---	---		
Pressure (kPa)	---	---	---		
Molar Flow (kgmole/h)	---	---	---		
Mass Flow (kg/h)	---	---	---		
Std Ideal Liq Vol Flow (m3/h)	---	---	---		
Heat Flow (MW)	103.856396	349.963110	20.4667134		
Molar Enthalpy (kJ/kgmole)	---	---	---		
Comp Mass Frac (CuCl*)	---	---	---		
Comp Mass Frac (HCl)	---	---	---		
Comp Mass Frac (Helium)	---	---	---		
Comp Mass Frac (CuO.CuCl2*)	---	---	---		
Comp Mass Frac (CuCl2*)	---	---	---		
Comp Mass Frac (H2O)	---	---	---		
Comp Mass Frac (Hydrogen)	---	---	---		
Comp Mass Frac (Oxygen)	---	---	---		
Comp Mass Frac (Nitrogen)	---	---	---		
Comp Mole Frac (CuCl*)	---	---	---		
Comp Mole Frac (HCl)	---	---	---		
Comp Mole Frac (Helium)	---	---	---		
Comp Mole Frac (CuO.CuCl2*)	---	---	---		
Comp Mole Frac (CuCl2*)	---	---	---		
Comp Mole Frac (H2O)	---	---	---		
Comp Mole Frac (Hydrogen)	---	---	---		
Comp Mole Frac (Oxygen)	---	---	---		
Comp Mole Frac (Nitrogen)	---	---	---		

Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc Level
CRV-101	Conversion Reactor	10- H2O 6- CuCl2 hot QR2	11- CuCl2 19- HCl + H2O QR2	No	500.0 *
CRV-102	Conversion Reactor	13- CuOCuCl2 QR3	17- CuCl-l 14- Oxygen QR3	No	500.0 *
CRV-100	Conversion Reactor	1- HCl 2- CuCl QNA1	4- CuCl2 3-H2 QNA1	No	500.0 *
E-105	Cooler	41- He	42- He QR3	No	500.0 *
E-108	Cooler	43- He	44- He Q CuCl2 heat	No	500.0 *
E-109	Cooler	45- He for electricity	46- He Qe-needed	No	500.0 *
E-112	Cooler	42- He	43- He QR2	No	500.0 *
E-111	Cooler	51	52 Qth	No	500.0 *
E-107	Cooler	21	22- Liquid HCl + H2O QNA2	No	500.0 *
E-106	Heater	5.1- CuCl2 dry Q CuCl2 heat	6- CuCl2 hot	No	500.0 *
E-102	Heater	20- Recycle Qwaste	21	No	500.0 *
V-100	Tank	4- CuCl2 Qdryer	5- CuCl2 dry 7- H2O Vap Qdryer	No	500.0 *

* Specified by user.

Unit Ops (continued)

Operation Name	Operation Type	Feeds	Products	Ignored	Calc Level
E-101	Heat Exchanger	11- CuCl2	12- CuOCuCl2	No	500.0 *
		14- Oxygen	15- O2 cool		
E-104	Heat Exchanger	17- CuCl-l	18- CuCl cooled	No	500.0 *
		26- Air	27- Air		
E-103	Heat Exchanger	12- CuOCuCl2	13- CuOCuCl2	No	500.0 *
		27- Air	28- Air		
E-100	Heat Exchanger	9	10- H2O	No	500.0 *
		28- Air	29- Air		
E-110	Heat Exchanger	19- HCl + H2O	20- Recycle	No	500.0 *
		24- Air	25- Air		
E-114	Heat Exchanger	30- Air	31- Air	No	500.0 *
		8- Extra Water	9		
E-115	Heat Exchanger	5- CuCl2 dry	5.1- CuCl2 dry	No	500.0 *
		15- O2 cool	16- O2 cool		
MIX-101	Mixer	25- Air	30- Air	No	500.0 *
		29- Air			
MIX-100	Mixer	44- He	47- He Out	No	500.0 *
		46- He			
TEE-100	Tee	50	40- He In	No	500.0 *
			51		
TEE-101	Tee	40- He In	41- He	No	500.0 *
			45- He for electricity		
SET-3	Set			No	500.0 *
SET-2	Set			No	500.0 *
SET-1	Set			No	500.0 *
SET-4	Set			No	500.0 *
P-100	Pump	22- Liquid HCl + H2O	23	No	500.0 *
		Q pump			

Table A-7: Mass and Energy Balance for the Kemp Model with a compressor

Streams

Fluid Pkg: All

Name		1- HCl	2- CuCl	3-H2	4- CuCl2	5- CuCl2 dry
Vapour Fraction		0.6756	0.0000	1.0000	0.0000	0.0000
Temperature	(C)	70.00 *	70.00 *	70.00	70.00 *	82.00
Pressure	(kPa)	2400 *	2400 *	2400	2400	50.00 *
Molar Flow	(kgmole/h)	6210.0	4140.0	2099.3	6180.7	4140.0
Mass Flow	(kg/h)	188239	409856	4704.07	593395	556635
Std Ideal Liq Vol Flow	(m3/h)	210.8	99.00	60.26	200.6	163.7
Heat Flow	(MW)	-267.405943	-152.727522	-1.23339465	-392.778236	-231.440727
Molar Enthalpy	(kJ/kgmole)	-1.550e+005	-1.328e+005	-2115	-2.288e+005	-2.013e+005
Comp Mass Frac (CuCl*)		0.0000 *	1.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (HCl)		0.8019 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (Helium)		0.0000 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (CuO.CuCl2*)		0.0000 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (CuCl2*)		0.0000 *	0.0000 *	0.0000	0.9380	1.0000
Comp Mass Frac (H2O)		0.1981 *	0.0000 *	0.1129	0.0619	0.0000
Comp Mass Frac (Hydrogen)		0.0000 *	0.0000 *	0.8871	0.0000	0.0000
Comp Mass Frac (Oxygen)		0.0000 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (Nitrogen)		0.0000 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl*)		0.0000 *	1.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (HCl)		0.6667 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (Helium)		0.0000 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (CuO.CuCl2*)		0.0000 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl2*)		0.0000 *	0.0000 *	0.0000	0.6698	1.0000
Comp Mole Frac (H2O)		0.3333 *	0.0000 *	0.0140	0.3301	0.0000
Comp Mole Frac (Hydrogen)		0.0000 *	0.0000 *	0.9860	0.0000	0.0000
Comp Mole Frac (Oxygen)		0.0000 *	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (Nitrogen)		0.0000 *	0.0000 *	0.0000	0.0000	0.0000

Name		5.1	6- CuCl2 hot	7- H2O Vap	8 Water	9
Vapour Fraction		0.0000	0.0000	1.0000	0.0000	1.0000
Temperature	(C)	110.6	370.0 *	82.00 *	25.00 *	250.0 *
Pressure	(kPa)	50.00	50.00	50.00 *	101.3 *	50.00 *
Molar Flow	(kgmole/h)	4140.0	4140.0	2040.7	4140.0 *	4140.0
Mass Flow	(kg/h)	556635	556635	36760.3	74582.5	74582.5
Std Ideal Liq Vol Flow	(m3/h)	163.7	163.7	36.84	74.73	74.73
Heat Flow	(MW)	-228.783686	-204.722188	-135.992486	-329.153766	-269.191060
Molar Enthalpy	(kJ/kgmole)	-1.989e+005	-1.780e+005	-2.399e+005	-2.862e+005	-2.341e+005
Comp Mass Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (HCl)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (Helium)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (CuCl2*)		1.0000	1.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (H2O)		0.0000	0.0000	1.0000	1.0000 *	1.0000
Comp Mass Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (HCl)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (Helium)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (CuCl2*)		1.0000	1.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (H2O)		0.0000	0.0000	0.9999	1.0000 *	1.0000
Comp Mole Frac (Hydrogen)		0.0000	0.0000	0.0001	0.0000 *	0.0000
Comp Mole Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000 *	0.0000

* Specified by user.

Streams (continued)

Fluid Pkg: All

Name		10- H2O	11- CuOCuCl2	12- CuOCuCl2	13- CuOCuCl2	14- Oxygen
Vapour Fraction		1.0000	0.0000	0.0000	0.0000	1.0000
Temperature	(C)	400.0 *	370.0 *	388.0 *	430.0 *	530.0 *
Pressure	(kPa)	50.00 *	50.00	101.3 *	101.3	101.3
Molar Flow	(kgmole/h)	4140.0	2070.0	2070.0	2070.0	1035.0
Mass Flow	(kg/h)	74582.5	442977	442977	442977	33120.0
Std Ideal Liq Vol Flow	(m3/h)	74.73	108.6	108.6	108.6	29.11
Heat Flow	(MW)	-262.891450	-196.522991	-195.149511	-191.916940	4.57980338
Molar Enthalpy	(kJ/kgmole)	-2.286e+005	-3.418e+005	-3.394e+005	-3.338e+005	1.593e+004
Comp Mass Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Helium)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuO.CuCl2*)		0.0000	1.0000	1.0000	1.0000	0.0000
Comp Mass Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (H2O)		1.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	1.0000
Comp Mass Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Helium)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuO.CuCl2*)		0.0000	1.0000	1.0000	1.0000	0.0000
Comp Mole Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (H2O)		1.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	1.0000
Comp Mole Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000

Name		15- O2 cool	16- O2 cool	17- CuCl-l	18- CuCl cooled	19- HCl + H2O
Vapour Fraction		1.0000	1.0000	0.0000	0.0000	1.0000
Temperature	(C)	385.8	90.00 *	530.0	70.00 *	370.0
Pressure	(kPa)	101.3	101.3	101.3	2400 *	50.00
Molar Flow	(kgmole/h)	1035.0	1035.0	4140.0	4140.0	6210.0
Mass Flow	(kg/h)	33120.0	33120.0	409859	409859	188239
Std Ideal Liq Vol Flow	(m3/h)	29.11	29.11	99.00	99.00	210.8
Heat Flow	(MW)	3.20632288	0.549280998	-105.594951	-152.728756	-226.516703
Molar Enthalpy	(kJ/kgmole)	1.115e+004	1911	-9.182e+004	-1.328e+005	-1.313e+005
Comp Mass Frac (CuCl*)		0.0000	0.0000	1.0000	1.0000	0.0000
Comp Mass Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.8019
Comp Mass Frac (Helium)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (H2O)		0.0000	0.0000	0.0000	0.0000	0.1981
Comp Mass Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Oxygen)		1.0000	1.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl*)		0.0000	0.0000	1.0000	1.0000	0.0000
Comp Mole Frac (HCl)		0.0000	0.0000	0.0000	0.0000	0.6667
Comp Mole Frac (Helium)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (H2O)		0.0000	0.0000	0.0000	0.0000	0.3333
Comp Mole Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Oxygen)		1.0000	1.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.0000

Streams (continued)

Fluid Pkg: All

Name		20- Recycle	21	22- Liquid HCl + H2O	23	24- Air
Vapour Fraction		0.7834	1.0000	0.0000 *	0.0000	1.0000
Temperature	(C)	40.30	70.00 *	-95.85	-95.37	25.00 *
Pressure	(kPa)	50.00	50.00 *	50.00	2400 *	200.0 *
Molar Flow	(kgmole/h)	6210.0	6210.0	6210.0	6210.0	20700
Mass Flow	(kg/h)	188239	188239	188239	188239	595443
Std Ideal Liq Vol Flow	(m3/h)	210.8	210.8	210.8	210.8	693.3
Heat Flow	(MW)	-260.809451	-242.895108	-299.937498	-299.800107	-9.22879085e-002
Molar Enthalpy	(kJ/kgmole)	-1.512e+005	-1.408e+005	-1.739e+005	-1.738e+005	-16.05
Comp Mass Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (HCl)		0.8019	0.8019	0.8019	0.8019	0.0000 *
Comp Mass Frac (Helium)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (H2O)		0.1981	0.1981	0.1981	0.1981	0.0000 *
Comp Mass Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mass Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	0.2100 *
Comp Mass Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.7900 *
Comp Mole Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (HCl)		0.6667	0.6667	0.6667	0.6667	0.0000 *
Comp Mole Frac (Helium)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (H2O)		0.3333	0.3333	0.3333	0.3333	0.0000 *
Comp Mole Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	0.1888 *
Comp Mole Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	0.8112 *

Name		25- Air	26- Air	27- Air	28- Air	29- Air
Vapour Fraction		1.0000	1.0000	1.0000	1.0000	1.0000
Temperature	(C)	225.0 *	25.00 *	490.0 *	459.3	399.1
Pressure	(kPa)	195.0	200.0 *	195.0	190.0	185.0
Molar Flow	(kgmole/h)	20700	11936	11936	11936	11936
Mass Flow	(kg/h)	595443	343334	343334	343334	343334
Std Ideal Liq Vol Flow	(m3/h)	693.3	399.7	399.7	399.7	399.7
Heat Flow	(MW)	34.2004604	-5.32135117e-002	47.0805916	43.8480212	37.5484110
Molar Enthalpy	(kJ/kgmole)	5948	-16.05	1.420e+004	1.323e+004	1.133e+004
Comp Mass Frac (CuCl*)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (HCl)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (Helium)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (CuO.CuCl2*)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (CuCl2*)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (H2O)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (Hydrogen)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mass Frac (Oxygen)		0.2100	0.2100 *	0.2100	0.2100	0.2100
Comp Mass Frac (Nitrogen)		0.7900	0.7900 *	0.7900	0.7900	0.7900
Comp Mole Frac (CuCl*)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (HCl)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (Helium)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (CuO.CuCl2*)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl2*)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (H2O)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (Hydrogen)		0.0000	0.0000 *	0.0000	0.0000	0.0000
Comp Mole Frac (Oxygen)		0.1888	0.1888 *	0.1888	0.1888	0.1888
Comp Mole Frac (Nitrogen)		0.8112	0.8112 *	0.8112	0.8112	0.8112

* Specified by user.

Streams (continued)

Fluid Pkg: All

Name	30- Air	31- Air	32- Air compressed	40- He In	41- He In
Vapour Fraction	1.0000	1.0000	1.0000	1.0000	1.0000
Temperature (C)	289.3	69.76	83.56	720.8 *	720.8
Pressure (kPa)	185.0	180.0	200.0 *	3000 *	3000
Molar Flow (kgmole/h)	32635	32635	32635	1.4389e+005	71946
Mass Flow (kg/h)	938777	938777	938777	576000 *	288000
Std Ideal Liq Vol Flow (m3/h)	1093	1093	1093	4643	2321
Heat Flow (MW)	71.7488714	11.7861656	15.4707282	578.639862	289.319931
Molar Enthalpy (kJ/kgmole)	7915	1300	1707	1.448e+004	1.448e+004
Comp Mass Frac (CuCl*)	0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (HCl)	0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (Helium)	0.0000	0.0000	0.0000	1.0000 *	1.0000
Comp Mass Frac (CuO.CuCl2*)	0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (CuCl2*)	0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (H2O)	0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (Hydrogen)	0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mass Frac (Oxygen)	0.2100	0.2100	0.2100	0.0000 *	0.0000
Comp Mass Frac (Nitrogen)	0.7900	0.7900	0.7900	0.0000 *	0.0000
Comp Mole Frac (CuCl*)	0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (HCl)	0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (Helium)	0.0000	0.0000	0.0000	1.0000 *	1.0000
Comp Mole Frac (CuO.CuCl2*)	0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (CuCl2*)	0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (H2O)	0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (Hydrogen)	0.0000	0.0000	0.0000	0.0000 *	0.0000
Comp Mole Frac (Oxygen)	0.1888	0.1888	0.1888	0.0000 *	0.0000
Comp Mole Frac (Nitrogen)	0.8112	0.8112	0.8112	0.0000 *	0.0000

Name	42	43	44	45- He for Electricity	46
Vapour Fraction	1.0000	1.0000	1.0000	1.0000	1.0000
Temperature (C)	502.2	395.0	337.2	720.8	264.3
Pressure (kPa)	3000	3000	3000	3000	3000
Molar Flow (kgmole/h)	71946	71946	71946	71946	71946
Mass Flow (kg/h)	288000	288000	288000	288000	288000
Std Ideal Liq Vol Flow (m3/h)	2321	2321	2321	2321	2321
Heat Flow (MW)	198.418138	153.844194	129.782696	289.319931	99.4821738
Molar Enthalpy (kJ/kgmole)	9928	7698	6494	1.448e+004	4978
Comp Mass Frac (CuCl*)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (HCl)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Helium)	1.0000	1.0000	1.0000	1.0000	1.0000
Comp Mass Frac (CuO.CuCl2*)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (CuCl2*)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (H2O)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Hydrogen)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Oxygen)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mass Frac (Nitrogen)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl*)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (HCl)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Helium)	1.0000	1.0000	1.0000	1.0000	1.0000
Comp Mole Frac (CuO.CuCl2*)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (CuCl2*)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (H2O)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Hydrogen)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Oxygen)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Nitrogen)	0.0000	0.0000	0.0000	0.0000	0.0000

* Specified by user.

Streams (continued)

Fluid Pkg: All

Name		47- He Out	50	51	52	Q comp
Vapour Fraction		1.0000	1.0000	1.0000	1.0000	---
Temperature	(C)	300.8	720.8	720.8	300.8	---
Pressure	(kPa)	3000	3000	3000	3000	---
Molar Flow	(kgmole/h)	1.4389e+005	2.8779e+005	1.4389e+005	1.4389e+005	---
Mass Flow	(kg/h)	576000	1.15200e+006	576000	576000	---
Std Ideal Liq Vol Flow	(m3/h)	4643	9286	4643	4643	---
Heat Flow	(MW)	229.264870	1157.27972	578.639862	229.264870	3.68456259
Molar Enthalpy	(kJ/kgmole)	5736	1.448e+004	1.448e+004	5736	---
Comp Mass Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	---
Comp Mass Frac (HCl)		0.0000	0.0000	0.0000	0.0000	---
Comp Mass Frac (Helium)		1.0000	1.0000	1.0000	1.0000	---
Comp Mass Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	---
Comp Mass Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	---
Comp Mass Frac (H2O)		0.0000	0.0000	0.0000	0.0000	---
Comp Mass Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	---
Comp Mass Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	---
Comp Mass Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	---
Comp Mole Frac (CuCl*)		0.0000	0.0000	0.0000	0.0000	---
Comp Mole Frac (HCl)		0.0000	0.0000	0.0000	0.0000	---
Comp Mole Frac (Helium)		1.0000	1.0000	1.0000	1.0000	---
Comp Mole Frac (CuO.CuCl2*)		0.0000	0.0000	0.0000	0.0000	---
Comp Mole Frac (CuCl2*)		0.0000	0.0000	0.0000	0.0000	---
Comp Mole Frac (H2O)		0.0000	0.0000	0.0000	0.0000	---
Comp Mole Frac (Hydrogen)		0.0000	0.0000	0.0000	0.0000	---
Comp Mole Frac (Oxygen)		0.0000	0.0000	0.0000	0.0000	---
Comp Mole Frac (Nitrogen)		0.0000	0.0000	0.0000	0.0000	---

Name		Q CuCl2 heat	Q pump	Q waste extra	Qdryer	Qe-needed
Vapour Fraction		---	---	---	---	---
Temperature	(C)	---	---	---	---	---
Pressure	(kPa)	---	---	---	---	---
Molar Flow	(kgmole/h)	---	---	---	---	---
Mass Flow	(kg/h)	---	---	---	---	---
Std Ideal Liq Vol Flow	(m3/h)	---	---	---	---	---
Heat Flow	(MW)	24.0614972	0.137391332	17.9143437	25.3450228	189.837757 *
Molar Enthalpy	(kJ/kgmole)	---	---	---	---	---
Comp Mass Frac (CuCl*)		---	---	---	---	---
Comp Mass Frac (HCl)		---	---	---	---	---
Comp Mass Frac (Helium)		---	---	---	---	---
Comp Mass Frac (CuO.CuCl2*)		---	---	---	---	---
Comp Mass Frac (CuCl2*)		---	---	---	---	---
Comp Mass Frac (H2O)		---	---	---	---	---
Comp Mass Frac (Hydrogen)		---	---	---	---	---
Comp Mass Frac (Oxygen)		---	---	---	---	---
Comp Mass Frac (Nitrogen)		---	---	---	---	---
Comp Mole Frac (CuCl*)		---	---	---	---	---
Comp Mole Frac (HCl)		---	---	---	---	---
Comp Mole Frac (Helium)		---	---	---	---	---
Comp Mole Frac (CuO.CuCl2*)		---	---	---	---	---
Comp Mole Frac (CuCl2*)		---	---	---	---	---
Comp Mole Frac (H2O)		---	---	---	---	---
Comp Mole Frac (Hydrogen)		---	---	---	---	---
Comp Mole Frac (Oxygen)		---	---	---	---	---
Comp Mole Frac (Nitrogen)		---	---	---	---	---

* Specified by user.

Streams (continued)

Fluid Pkg: All

Name		QNA1	QNA2	QR2	QR3	Qth
Vapour Fraction		---	---	---	---	---
Temperature	(C)	---	---	---	---	---
Pressure	(kPa)	---	---	---	---	---
Molar Flow	(kgmole/h)	---	---	---	---	---
Mass Flow	(kg/h)	---	---	---	---	---
Std Ideal Liq Vol Flow	(m3/h)	---	---	---	---	---
Heat Flow	(MW)	26.1218269	57.0423909	44.5739445	90.9017926	349.374991
Molar Enthalpy	(kJ/kgmole)	---	---	---	---	---
Comp Mass Frac (CuCl*)		---	---	---	---	---
Comp Mass Frac (HCl)		---	---	---	---	---
Comp Mass Frac (Helium)		---	---	---	---	---
Comp Mass Frac (CuO.CuCl2*)		---	---	---	---	---
Comp Mass Frac (CuCl2*)		---	---	---	---	---
Comp Mass Frac (H2O)		---	---	---	---	---
Comp Mass Frac (Hydrogen)		---	---	---	---	---
Comp Mass Frac (Oxygen)		---	---	---	---	---
Comp Mass Frac (Nitrogen)		---	---	---	---	---
Comp Mole Frac (CuCl*)		---	---	---	---	---
Comp Mole Frac (HCl)		---	---	---	---	---
Comp Mole Frac (Helium)		---	---	---	---	---
Comp Mole Frac (CuO.CuCl2*)		---	---	---	---	---
Comp Mole Frac (CuCl2*)		---	---	---	---	---
Comp Mole Frac (H2O)		---	---	---	---	---
Comp Mole Frac (Hydrogen)		---	---	---	---	---
Comp Mole Frac (Oxygen)		---	---	---	---	---
Comp Mole Frac (Nitrogen)		---	---	---	---	---

Unit Ops

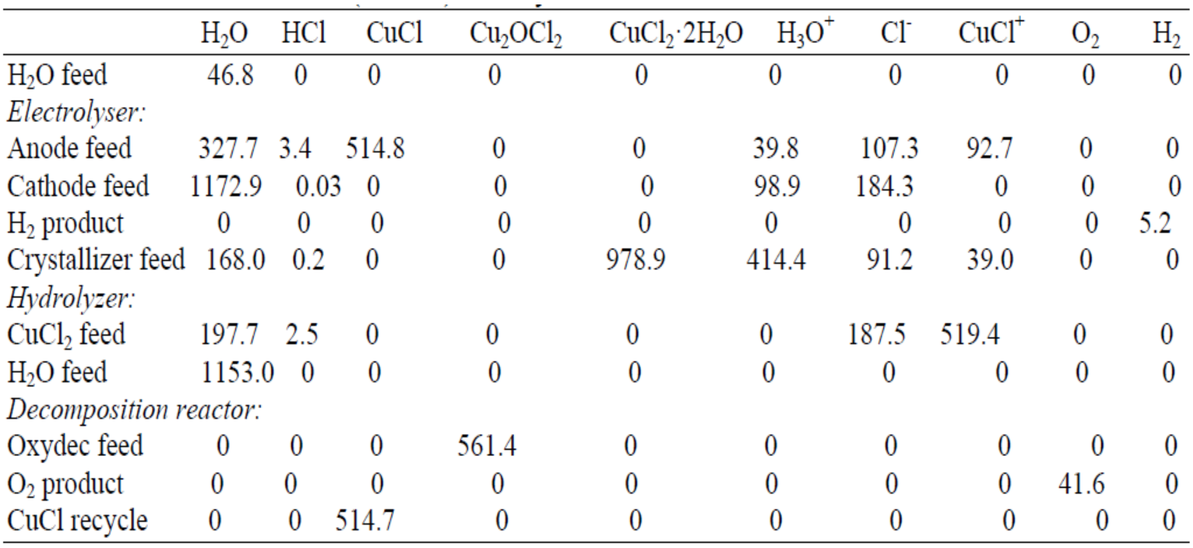
Operation Name	Operation Type	Feeds	Products	Ignored	Calc Level
CRV-101	Conversion Reactor	10- H2O 6- CuCl2 hot QR2	11- CuOCuCl2 19- HCl + H2O QR2	No	500.0 *
CRV-102	Conversion Reactor	13- CuOCuCl2 QR3	17- CuCl-l 14- Oxygen QR3	No	500.0 *
CRV-100	Conversion Reactor	1- HCl 2- CuCl QNA1	4- CuCl2 3-H2 QNA1	No	500.0 *
E-105	Cooler	41- He In	42 QR3	No	500.0 *
E-108	Cooler	43	44 Q CuCl2 heat	No	500.0 *
E-109	Cooler	45- He for Electricity	46 Qe-needed	No	500.0 *
E-112	Cooler	42	43 QR2	No	500.0 *
E-111	Cooler	51	52 Qth	No	500.0 *
E-107	Cooler	21	22- Liquid HCl + H2O QNA2	No	500.0 *
E-106	Heater	5.1 Q CuCl2 heat	6- CuCl2 hot	No	500.0 *
E-102	Heater	20- Recycle Q waste extra	21	No	500.0 *
V-100	Tank	4- CuCl2 Qdryer	5- CuCl2 dry 7- H2O Vap Qdryer	No	500.0 *

* Specified by user.

Unit Ops (continued)

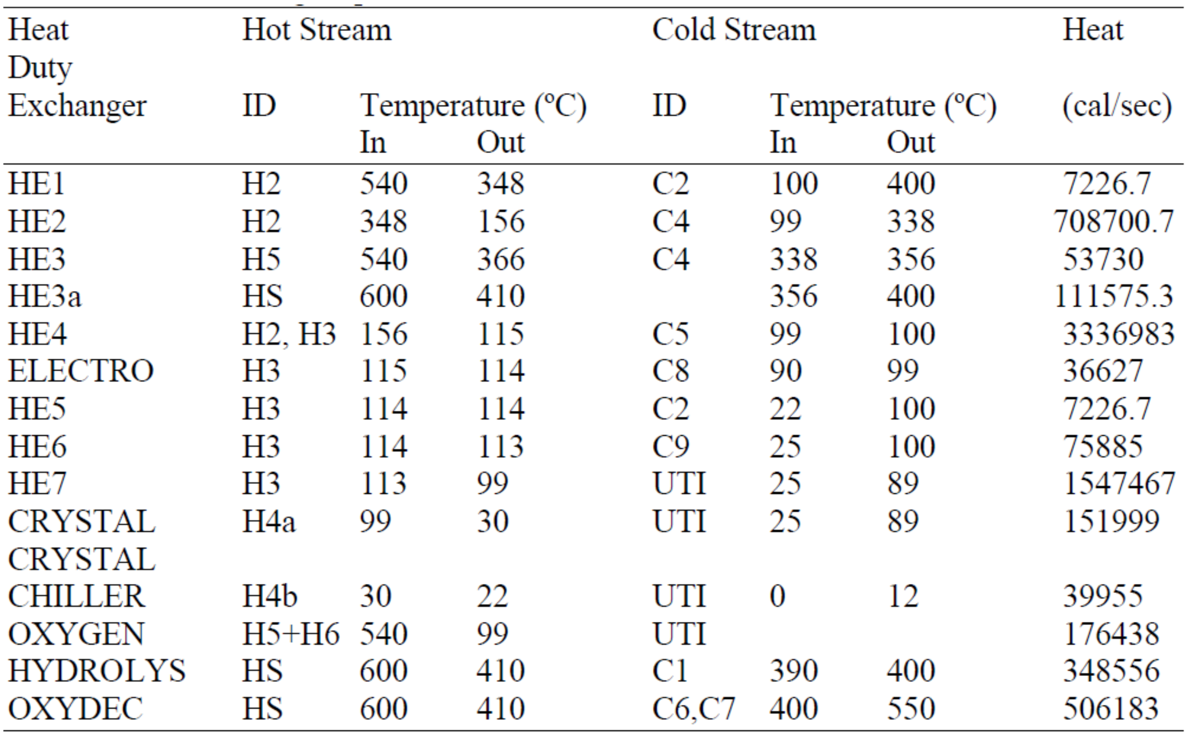
Operation Name	Operation Type	Feeds	Products	Ignored	Calc Level
E-101	Heat Exchanger	11- CuOCuCl2 14- Oxygen	12- CuOCuCl2 15- O2 cool	No	500.0 *
E-104	Heat Exchanger	17- CuCl-l 26- Air	18- CuCl cooled 27- Air	No	500.0 *
E-103	Heat Exchanger	12- CuOCuCl2 27- Air	13- CuOCuCl2 28- Air	No	500.0 *
E-100	Heat Exchanger	9 28- Air	10- H2O 29- Air	No	500.0 *
E-110	Heat Exchanger	19- HCl + H2O 24- Air	20- Recycle 25- Air	No	500.0 *
E-114	Heat Exchanger	30- Air 8 Water	31- Air 9	No	500.0 *
E-115	Heat Exchanger	5- CuCl2 dry 15- O2 cool	5.1 16- O2 cool	No	500.0 *
MIX-101	Mixer	25- Air 29- Air	30- Air	No	500.0 *
MIX-100	Mixer	44 46	47- He Out	No	500.0 *
TEE-100	Tee	50	40- He In 51	No	500.0 *
TEE-101	Tee	40- He In	41- He In 45- He for Electricity	No	500.0 *
SET-3	Set			No	500.0 *
SET-2	Set			No	500.0 *
SET-1	Set			No	500.0 *
SET-4	Set			No	500.0 *
P-100	Pump	22- Liquid HCl + H2O Q pump	23	No	500.0 *
K-100	Compressor	31- Air Q comp	32- Air compressed	No	500.0 *

Table A-8: Mass balance for the Aspen flowsheet of the Canadian model with mass flow in MT/h (Ferrandon et al, sa)



	H_2O	HCl	CuCl	Cu_2OCl_2	$CuCl_2{\cdot}2H_2O$	H_3O^+	Cl^-	$CuCl^+$	O_2	H_2
H_2O feed	46.8	0	0	0	0	0	0	0	0	0
Electrolyser:										
Anode feed	327.7	3.4	514.8	0	0	39.8	107.3	92.7	0	0
Cathode feed	1172.9	0.03	0	0	0	98.9	184.3	0	0	0
H_2 product	0	0	0	0	0	0	0	0	0	5.2
Crystallizer feed	168.0	0.2	0	0	978.9	414.4	91.2	39.0	0	0
Hydrolyzer:										
$CuCl_2$ feed	197.7	2.5	0	0	0	0	187.5	519.4	0	0
H_2O feed	1153.0	0	0	0	0	0	0	0	0	0
Decomposition reactor:										
Oxydec feed	0	0	0	561.4	0	0	0	0	0	0
O_2 product	0	0	0	0	0	0	0	0	41.6	0
CuCl recycle	0	0	514.7	0	0	0	0	0	0	0

Table A-9: Energy balance of the Aspen flowsheet of the Canadian model, energy shown in cal/s, HS = Heat source, UTI = Utilities (Ferrandon *et al*, sa).



Heat Exchanger	Hot Stream			Cold Stream			Heat Duty
	ID	Temperature (°C)		ID	Temperature (°C)		(cal/sec)
		In	Out		In	Out	
HE1	H2	540	348	C2	100	400	7226.7
HE2	H2	348	156	C4	99	338	708700.7
HE3	H5	540	366	C4	338	356	53730
HE3a	HS	600	410		356	400	111575.3
HE4	H2, H3	156	115	C5	99	100	3336983
ELECTRO	H3	115	114	C8	90	99	36627
HE5	H3	114	114	C2	22	100	7226.7
HE6	H3	114	113	C9	25	100	75885
HE7	H3	113	99	UTI	25	89	1547467
CRYSTAL	H4a	99	30	UTI	25	89	151999
CRYSTAL CHILLER	H4b	30	22	UTI	0	12	39955
OXYGEN	H5+H6	540	99	UTI			176438
HYDROLYS	HS	600	410	C1	390	400	348556
OXYDEC	HS	600	410	C6,C7	400	550	506183