Title
Integration of an Absorption Chiller with a High Temperature Fuel Cell for Polygeneration of Cooling, Heating, Power, and Hydrogen

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Integration of an Absorption Chiller with a High Temperature Fuel Cell for Polygeneration of Cooling, Heating, Power, and Hydrogen

THESIS

Submitted in partial satisfaction of the requirements for the degree of

MASTER OF SCIENCE
In Mechanical Engineering

By
Derek McVay

Thesis Committee:
Professor Jack Brouwer
Professor Scott Samuelsen
Professor Faryar Jabbari
DEDICATION

This work is dedicated to my parents, Jim and Linda, for raising and shaping me into the person I would become. It is dedicated to my lovely wife, Jaclyn, for loving me and supporting me throughout my seemingly never-ending time as a student. This is also dedicated to my children, Cora and Georgia; I want to provide a better future for them, for their generation, and future generations.
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NOMENCLATURE

BOP    Balance of Plant
CCHP   Combined cooling heating and power
COP    Coefficient of performance
HHV    Higher-heating value
hr     Hour
HSU    Hydrogen separation unit
HTFC   High temperature fuel cell
kg     Kilogram
kW     Kilowatt
kWh    Kilowatt-hour
LHV    Lower-heating value
MEA    Membrane-electrode assembly
MCFC   Molten carbonate fuel cell
MW     Megawatt
PSA    Pressure swing adsorption
SMR    Steam methane reaction
SOFC   Solid oxide fuel cell
TPB    Triple-phase boundary
WSGR   Water gas shift reaction
LIST OF SYMBOLS

$Q$  Heat

$\mu$  chemical potential

$a$  activity

$A$  amperes

$\alpha$  electron transfer coefficient

$C$  chemical product

$c$  concentration

$D$  Diffusivity

$E$  Energy flow

$\varepsilon$  effectiveness

$E_a$  activation energy

$E_o$  open circuit voltage

$f$  fuel

$F$  Faraday's constant

$g$  Gibbs free energy

$H$  enthalpy

$H_2$  hydrogen product

$I$  electric current

$j$  current density

$J$  diffusion flux

$\dot{n}$  molar flow rate
P electric power
$P$ pressure
$p$ partial pressure
$q$ specific heat
$Q$ heat
$R$ gas constant
$S$ entropy
$s$ seconds
$T$ temperature
$U_f$ fuel utilization factor
$U_{O2}$ air utilization factor
$V$ voltage
$W$ work
$w$ specific work
$z$ number of electrons released during oxidation
$\eta$ efficiency
$\dot{m}$ Mass flow rate
$j_o$ exchange current density
ABSTRACT OF THE THESIS

Integration of an Absorption Chiller with a High Temperature Fuel Cell for Polygeneration of Cooling, Heating, Power, and Hydrogen

By

Derek McVay

Master of Science in Mechanical and Aerospace Engineering

University of California, Irvine, 2014

Professor Jacob Brouwer, Chair

As awareness of greenhouse gas and harmful pollutant emissions rises, interest is also growing to curb the trend in an effort to reduce the harmful impacts that these emissions create. A large contributor to these emissions is stationary power generation sources which are typically powered by traditional heat engines. High temperature fuel cells provide an alternative solution to power generation which can have higher efficiency than heat engines, thus reducing overall harmful emissions. Fuel cells are also capable of using renewable streams of fuel so that the greenhouse gas emissions are completely negated.

Different system configurations based upon a solid oxide fuel cell power plant were modeled in bulk using Aspen Plus. The three configurations modeled were: a baseline Tri-Generation system that produces combined heating, hydrogen, and power; a Quad-Generation system that produces combined cooling, heating, hydrogen, and power; a Tri-Generation system that produces combined heating, hydrogen, and power that is supplemented with an absorption chiller within the hydrogen booster.

A parametric study was performed on the three systems in order to find any efficiency or operating gains compared to the baseline Tri-Generation system. Electricity and hydrogen
generation efficiency were found to be greatest at the lowest evaluated fuel utilization of 0.6. System efficiency for the baseline Tri-Generation was the highest at 0.6 fuel utilization and decreased with increasing fuel utilization. Varying levels of power capacity had little effect on the system efficiency. Quad-Generation efficiency depended upon the coefficient of performance (COP). At a low COP of 1.1, overall system efficiency was lower than the baseline for a given fuel utilization. At a COP of 1.4, the overall efficiency was higher than the baseline and the impact of fuel utilization was reduced. The chiller supplemented Tri-Generation system also had lower system efficiency than the baseline; however, the impact of increased fuel utilization was reduced. For a given utilization, the efficiency stayed relatively unchanged. The result of unchanged efficiency as a function of fuel utilization for the Quad-Generation and the supplemented Tri-Generation systems suggests that these systems can be operated to follow dynamic loads without significant impact on system efficiency.
1. INTRODUCTION

1.1. Overview

The recent downward trend in the price of natural gas in addition to legislation aimed at reducing greenhouse gas emissions have spurred increased interest in the development of distributed power generation schemes [1]. High temperature fuel cells have become increasingly more common as a power generation technology that both takes advantage of natural gas and reduces greenhouse gas emissions as well as criteria pollutant emissions [2]. At power ratings typical for distributed generation, the electrical efficiency is typically greater than a comparable heat engine, such as a gas turbine. This means that an HTFC dispatched in place of a gas turbine can emit fewer greenhouse gases as well as criteria pollutants. Reduction in criteria pollutants is possible since the operating temperature of the fuel cell is below the temperature at which pollutants such as NOx, SOx, and particulate matter are generally formed [3].

As systems which directly generate electricity and heat, HTFCs have been increasingly considered for use in conjunction with other generation technologies. Some integration designs include heat engines (e.g., gas turbines, reciprocating engines, Stirling engines) as bottoming cycles to increase system power output and efficiency [4]. System efficiency is generally defined as the percentage of the amount of power delivered by a system with respect to the amount of energy input to the system. Systems with higher efficiency require less fuel input than systems with lower efficiency for a given amount of power. This reduces operating costs as well as emissions in general.
Power demand of almost any given scenario often includes some demand for cooling. Traditionally, electric chillers have been meeting that demand as a cheap and efficient method of providing cooling. During high cooling-demand periods, this can consume a high percentage of the power generator’s output which may require the operator to purchase power from the grid, thus increasing operating costs. Absorption chillers have been studied and deployed as a way to utilize heat in an exhaust stream of a heat engine or fuel cell, thus reducing the need for electric generation during cooling-demand periods. This scheme offers the potential to save on operating costs by increasing overall system efficiency and reducing electrical load [5]. Capital costs may also be reduced since the power generator would not need to be sized in order to provide electricity for all the cooling demand. Distributed generation systems that provide power and cooling also often provide heating and are referred to as combined cooling, heating, and power systems (CCHP).

More recently, high temperature fuel cells have been shown to provide conditions that favor the generation of hydrogen that can then be separated for use in proton exchange membrane fuel cells [6]. This has been referred to as Tri-Generation and operation in this manner enables a revenue stream in the form of hydrogen fuel for fuel cell vehicles. Lowering the fuel utilization and promoting internal steam-methane reformation increases electrical efficiency and eliminates the need for a separate reformation subsystem. A couple demonstration projects were capable of proving that the technology is feasible. A project in Anchorage, Alaska aimed to generate cheap hydrogen [7]. While another project in Fountain Valley, California demonstrated the operation of a Tri-Generation system on anaerobic digester gas from a waste water treatment plant [8]. The generation products of this system can be considered carbon neutral since the anaerobic digester gas was generated as a byproduct of waste water (e.g., sewage).
The current work aims to determine the feasibility of combining an absorption chiller with a Tri-Generation system. The purpose is to increase system efficiency and thus reduce operating costs while also creating an additional revenue stream in the form of hydrogen fuel for fuel cell vehicles. The system could potentially be fueled by natural gas, biogas, or syngas. This particular system configuration will be referred to as Quad-Generation throughout this work.

A Tri-Generation system uses an incorporated hydrogen separation unit which requires a significant amount of cooling for its processes. Previously, this cooling demand has been met by electric chillers. This current work will also consider replacing that electric chiller with an absorption chiller to reduce parasitic losses and understand its impact on the system’s performance.

1.2. Goal

The goal of the current research is to advance the concept and performance characteristics of Tri-Generation and Quad-Generation by understanding and describing the main challenges and benefits. The most effective way to approach this goal is to develop a computer model which simulates a potential Quad-Generation and chiller supplemented Tri-generation system configuration. The model should be verified and this will pave the way to propose how to incorporate a chiller with a Tri-Generation system, either for an exported product or for integration within the system itself.

1.3. Objectives

In order to meet the research goal stated above, the following objectives were established:

1. Create an integrated computer model of individual components of a baseline solid oxide fuel cell driven Tri-Generation system.
2. Create an integrated computer model of individual components of a Quad-Generation system based on the baseline Tri-Generation system.

3. Produce a steady-state model of the Quad-Generation system which incorporates the individual components of a Quad-Generation system.

4. Verify that the results of the model match literature results.

5. Determine the system configuration which optimizes electrical power and hydrogen production efficiency.

6. Determine the system configuration which optimizes electrical power, hydrogen production, and cooling output.

7. Implement the models with varying parameters in order to characterize performance.

2. BACKGROUND

2.1. Fuel cells

Fuel cell technology has been around for over 170 years, but recently that interest has grown enough in order to fully develop and understand the benefits available from implementing the technology on a wide scale. Fuel cell devices are capable of converting a constant stream of fuel directly into electricity without the need of turbines or any major moving parts. The following section discusses how fuel cells work and some of the motivating principles behind their operation.
2.1.1. Operation

The most basic type of fuel cell is one that runs off of pure hydrogen (fuel) and pure oxygen (oxidant). The fuel and oxidant are separated by the membrane-electrode assembly (MEA). The MEA is made up of two electrodes (the anode and cathode) and an electrolyte which is sandwiched between the two electrodes. The electrodes are permeable to gas so that the gases can make contact with the electrolyte. Points at which the gas, electrode, and electrolyte meet are points where an electrochemical reaction can occur which liberates an electron into or out of the electrode and an ion is transferred through the electrolyte. These points are called triple-phase boundaries (TPB). Figure 1 illustrates an active fuel cell for a proton-carrying electrolyte. The hydrogen splits, releasing two electrons into the anode while the hydrogen ions travel through the electrolyte. The ions then react with oxygen atoms and electrons in the cathode to form water. A voltage potential exists between the anode and cathode, this drives an electric current. The simplified reaction of the above combination of fuel and oxidant is as follows:

\[ H_2 + \frac{1}{2} O_2 \rightarrow H_2O \]  

Equation 2-1

Figure 1: Hydrogen fuel cell operating diagram http://ecofriend.com/wp-content/uploads/2012/07/top_3LfvZ_32853.jpg
Equation 2-1 is actually the overall reaction of the fuel cell and is made up of two half-reactions which occur at the anode and cathode TPBs.

Anode: \[ H_2 \rightarrow 2H^+ + 2e^- \] Equation 2-2

Cathode: \[ \frac{1}{2}O_2 + 2H^+ + 2e^- \rightarrow H_2O \] Equation 2-3

Equation 2-2 and Equation 2-3 are the two half reactions which occur at the anode and cathode respectively. Fuel cells are often categorized by the type of electrolyte they have and their operating temperature. The various materials that are used to make up different electrolytes often require different electrochemical reactions to take place. However, the characteristics of these different fuel cells are governed by fundamental principles.

2.1.2. Fundamental Thermodynamics

Since fuel cells rely on electrochemical reactions instead of combustion, they operate on different principles from heat engines, but can still be described from the first and second laws of thermodynamics. An important thermodynamic property for fuel cells is the Gibbs free energy which is a relation between enthalpy, temperature, and entropy as given by Equation 2-4:

\[ G = H - TS \] Equation 2-4

\[ H = U + PV \] Equation 2-5

Where \( G \) is the Gibbs free energy of the system, \( H \) is the enthalpy, \( T \) is temperature, \( S \) is the entropy, \( U \) is the internal energy, \( P \) is pressure, and \( V \) is the volume. In order to accurately describe a fuel cell system through Gibbs free energy it is necessary to hold temperature, pressure, and volume constant while the other properties must be considered as a difference
between products and reactants. This difference depends on the specific reaction taking place at either the anode or cathode.

Thus, differentiating Equation 2-4 and holding T constant, the equation becomes:

\[ dG = dH -TdS \] 

Equation 2-6

On a molar basis, Equation 2-6 can be rewritten as:

\[ \Delta \bar{g} = \Delta \bar{h} - T \Delta \bar{s} \] 

Equation 2-7

As stated, the change in enthalpy and the change in entropy are dependent on specific reactions and can be written in terms of their combined products and reactions:

\[ \Delta \bar{h}_{rxn} = \sum \nu_p \bar{h}_{products} - \sum \nu_r \bar{h}_{reactants} \] 

Equation 2-8

\[ \Delta \bar{s}_{rxn} = \sum \nu_p \bar{s}_{products} - \sum \nu_r \bar{s}_{reactants} \] 

Equation 2-9

Where \( \nu_p \) and \( \nu_r \) are respectively the product and reactant stoichiometric coefficients of the specific molecule involved in the reaction. Enthalpy and entropy can be rewritten as functions of specific heat and temperature since they cannot be measured directly:

\[ \bar{h}(T) = \bar{h}_f(T_0) + \int_{T_0}^{T} \bar{c}_p(T)dT \] 

Equation 2-10

\[ \bar{s}(T) = \bar{s}_f(T_0) + \int_{T_0}^{T} \frac{\bar{c}_p(T)}{T}dT \] 

Equation 2-11

Where \( T_0 \) is the reference temperature (298.15 K), \( \bar{h}_f(T_0) \) is the reference enthalpy at \( T_0 \), and \( \bar{s}_f(T_0) \) is the reference entropy at \( T_0 \). \( T \) is temperature, \( \bar{c}_p(T) \) is specific heat at \( T \). Rewriting the Gibbs free energy equation in terms of these properties:
\[ \Delta \bar{g}_{rxn} = \Delta \bar{h}_{rxn} - T \Delta \bar{s}_{rxn} \]  \hspace{1cm} \text{Equation 2-12}

The negative of the change in Gibbs free energy is equal to the reversible electric work a fuel cell can generate. The reversible efficiency of a fuel cell is the ratio of the Gibbs free energy and its enthalpy of reaction:

\[ \eta_{FCrev} = \frac{\Delta \bar{g}_{rxn}}{\Delta \bar{h}_{rxn}} = \frac{\Delta \bar{h}_{rxn} - T \Delta \bar{s}_{rxn}}{\Delta \bar{h}_{rxn}} \]  \hspace{1cm} \text{Equation 2-13}

Equation 2-13 represents the maximum theoretical efficiency limit of a fuel cell [9].

2.1.3. Reversible Voltage and Electrical Work

The maximum theoretical electrical work a fuel cell can generate is given by the negative of the change in Gibbs free energy.

\[ \bar{w}_e = -\Delta \bar{g}_{rxn} \]  \hspace{1cm} \text{Equation 2-14}

The power \((P)\) a fuel cell can generate depends on the reversible voltage \((V_{rev})\) and current \((I)\):

\[ P = V_{rev} \cdot I \]  \hspace{1cm} \text{Equation 2-15}

Power can also be expressed in terms of the molar flow of utilized fuel \(\dot{n}_f\) and the reversible work:

\[ P = \dot{n}_f \cdot \bar{w}_e = -\dot{n}_f \cdot \Delta \bar{g}_{rxn} \]  \hspace{1cm} \text{Equation 2-16}

Combining Equation 2-14, Equation 2-15, and Equation 2-16, voltage can be written as:

\[ V_{rev} = E_0 = -\frac{\dot{n}_f \cdot \Delta \bar{g}_{rxn}}{I} \]  \hspace{1cm} \text{Equation 2-17}

Current can be written as:
\[ I = z \cdot \dot{n}_f \cdot F \]  \hspace{1cm} \text{Equation 2-18}

Where \( F \) is Faraday’s constant \( \left( 96,485 \frac{c}{mol} \right) \) and \( z \) represents the number of electrons released from oxidation of a given fuel \( f \).

\[ z = \frac{\dot{n}_{e^-}}{\dot{n}_f} = \frac{\dot{n}_{e^-}}{U_f \cdot \dot{n}_{f,in} \cdot F} \]  \hspace{1cm} \text{Equation 2-19}

Where \( \dot{n}_{e^-} \) is the number of electrons released for the given fuel and reaction. \( U_f \) is the fuel utilization factor. Combining Equation 2-17, Equation 2-18, Equation 2-19 voltage can be expressed as:

\[ V_{rev} = E_0 = -\frac{\Delta \bar{G}_{rxn}}{z \cdot F} \]  \hspace{1cm} \text{Equation 2-20}

Equation 2-20 represents the fundamental equation for the open circuit voltage (OCV) of a fuel cell.

### 2.1.4. Nernst Potential from Concentration and Pressure Effects

Species concentrations, system pressure, and temperature affect the voltage of an operating fuel cell. The chemical potential, \( \mu \), is introduced in order to describe how the Gibbs free energy changes as a result of differing concentrations and pressures.

\[ \mu_i^\infty = \left( \frac{\partial G}{\partial n_i} \right)_{T,P,n_{j\neq i}} \]  \hspace{1cm} \text{Equation 2-21}

Where \( \mu \) is the chemical potential of species \( i \) in phase \( \infty \) with \( n_i \) representing the number of molecules of species. The chemical potential is related the activity of a given species \( a_i \).

\[ \mu_i = \mu_i^0 + RT\ln(a_i) \]  \hspace{1cm} \text{Equation 2-22}
Where \( \mu_i^0 \) is the reference chemical potential of species \( i \) at standard state conditions. The activity is a ratio of the species partial pressure \( p_i \) and the standard-state pressure \( p^0 \).

\[
a_i = \frac{p_i}{p^0}
\]

Equation 2-23

Combining Equation 2-21, Equation 2-22, and Equation 2-23 the change in Gibbs free energy can be expressed as

\[
dG = \sum_i \mu_i d n_i = \sum_i \left( \mu_i^0 + RT \ln(a_i) \right) d n_i
\]

Equation 2-24

The change in Gibbs free energy of formation can be written as

\[
\Delta \bar{g}_{rxn} = \Delta \bar{g}_{rxn}^0 + RT \ln \left( \frac{\prod a_{products}}{\prod a_{reactants}} \right)
\]

Equation 2-25

Substituting Equation 2-25 into Equation 2-20 the Nernst voltage \( V_{Nernst} \) is defined

\[
V_{Nernst} = E_0 - \frac{RT}{zF} \ln \left( \frac{\prod a_{products}}{\prod a_{reactants}} \right)
\]

Equation 2-26

The minus sign is turned positive if the activity of the reactants and products are flipped in accordance with properties of logarithms. If water is assumed to be in the form of steam, the Nernst voltage for a hydrogen fuel cell becomes

\[
V_{Nernst} = E_0 - \frac{RT}{2F} \ln \left( \frac{a_{H_2O}}{a_{H_2} a_{O_2}^2} \right)
\]

Equation 2-27

The Nernst voltage of a fuel cell is given as a function of the open circuit voltage and the activities of the species dominating the electrochemical reactions. The electrode of a fuel cell is considered an equipotential structure meaning that the voltage difference between the anode and
cathode electrodes at any given point will be the same across the entire surface. As a result, the current density must vary as a function of the species concentrations along the length of the fluid channel. An important factor in fuel cell operation is the utilization of fuel and oxidant. If 100% of fuel or oxidant is utilized inside the cell, then a portion of the cell will be starved, forcing the voltage difference of the entire cell to zero. Therefore, the utilization factor of fuel or oxidant must always be less than 100%. Other factors affect the operational voltage of the fuel cell and these are known as activation polarization, ohmic polarization, and concentration polarization.

\[ V_{\text{cell}} = V_{\text{Nernst}} - \eta_{\text{act}} - \eta_{\text{ohm}} - \eta_{\text{conc}} \]  
Equation 2-28

These losses are attributed to different phenomena, but each is directly related to the current density \( j \).

### 2.1.5. Activation Polarization

Activation polarization is computed on both the anode and cathode side of the fuel cell.

\[ \eta_{\text{act}} = \eta_{\text{act}}^{\text{an}} + \eta_{\text{act}}^{\text{cat}} \]  
Equation 2-29

The general Butler-Volmer (B-V) equation describes current density in terms of activation polarization and other factors for any given electrochemical reaction

\[ j = j_0 \left[ \exp \left( \frac{\alpha nF \eta_{\text{act}}}{RT} \right) - \exp \left( - \frac{(1 - \alpha)nF \eta_{\text{act}}}{RT} \right) \right] \]  
Equation 2-30

Where \( j \) is the current density, \( j_0 \) is the exchange current density, \( \alpha \) is the electron transfer coefficient (generally taken as 0.5), \( n \) is the number of electrons participating in the electrochemical reaction, \( F \) is Faraday’s constant, \( R \) is the universal gas constant, and \( T \) is the operating temperature of the cell [10].
The activation polarization, for modeling purposes, should be solved explicitly. As a result, alternatives to the B-V equation have been developed. For this work, a hyperbolic sine function approximation is used. This approximation is used since it has the widest applicability according to Noren and Hoffman [11]:

\[ \eta_{act} = \frac{RT}{\alpha n F} \sinh^{-1} \left( \frac{j}{2j_0} \right) \]  
Equation 2-31

Where the exchange current density \( j_0 \) is a function of the reacting species activities

\[ j_{0,an} = \gamma_{an}(a_{H_2})(a_{H_2O}) \exp \left( -\frac{E_{act,an}}{RT} \right) \]  
Equation 2-32

\[ j_{0,cath} = \gamma_{cath}(a_{O_2})^{0.25} \exp \left( -\frac{E_{act,cath}}{RT} \right) \]  
Equation 2-33

Where \( \gamma_i \) is the pre-exponential factor and \( E_{act,i} \) is the activation energy.

2.1.6. Ohmic Polarization

The flow of ions across the electrolyte also incurs voltage losses, this along with any resistance in the electrode and interconnects of a fuel cell are described by the ohmic polarization

\[ \eta_{ohm} = \sum_i j \cdot R_i \]  
Equation 2-34

Where \( R_i \) is the resistance of a specific structure (e.g., anode and cathode electrodes, electrolyte, and interconnects). For a fuel cell system, the ohmic losses are given by

\[ \eta_{ohm} = j(R_{an} + R_{elec} + R_{cath} + R_{IC}) \]  
Equation 2-35

The resistance of each structure is given by

\[ R_i = L_i \delta_i \]  
Equation 2-36
Where $L_i$ is the length through which the current travels through a structure and $\delta_i$ is the resistivity of the material.

2.1.7. Concentration Polarization

As fuel and oxidant are passing through the fluid channels at all times, electrochemical reactions are consuming and producing reactants and products. This creates a concentration gradient along the cross-section of the porous electrode which leads to diffusive transport. As current is increased, more fuel and oxidant are required to maintain the reactions at the TPB. The depletion of reactants affects the fuel cell voltage and is known as the concentration polarization or polarization due to mass transport. This can be expressed as a function of current density and diffusivity

$$j = nF J_{diff}$$

Equation 2-37

Where $J_{diff}$ is the diffusion flux of reactants to the catalyst layer or products away from the catalyst layer. Diffusive flux can be calculated by

$$J_{diff} = -D^{eff} \left( \frac{c^*_R - c^0_R}{\delta} \right)$$

Equation 2-38

Where $D^{eff}$ is the effective reactant diffusivity, $c^*_R$ and $c^0_R$ represent the reactant catalyst layer and bulk concentrations, respectively, and $\delta$ is the length of the diffusive layer (i.e., the thickness of the electrode) [12]. Another important relation is the current density at which starvation occurs. The limiting current density is the point at which the fuel or oxidant flow is not high enough to maintain reactions and the electrochemical reactions will cease

$$j_L = nF D^{eff} \frac{c^0_R}{\delta}$$

Equation 2-39
Where \( j_L \) is the limiting current density. Finally the concentration polarization can be expressed as

\[
\eta_{\text{conc}} = c \ln \left( \frac{j_L}{j_L - j} \right)
\]

Equation 2-40

Where \( c \) is a constant given by

\[
c = \left( \frac{RT}{nF} \right) \left( 1 + \frac{1}{\alpha} \right)
\]

Equation 2-41

2.2. Introduction to High Temperature Fuel Cells

High temperature fuel cells (HTFC) typically operate at temperatures between 750 °C and 1000 °C. There are two main types of fuel cells that operate in this temperature regime which are made up of different materials and operate differently. A unique advantage to the high temperature operation is that activation polarization is greatly diminished due to the dependence on temperature.

2.2.1. Molten Carbonate Fuel Cell

A molten carbonate fuel cell (MCFC) generally operates close to 800 °C. The electrolyte is made up of a carbonate electrolyte, that, when heated to temperature is in a molten state. This electrolyte is generally made up of lithium and potassium carbonates. The electrolyte is supported by a ceramic mesh which maintains the shape and integrity of the electrolyte during operation and down time. At temperature, the electrolyte is highly conducive to \( CO_2^- \) ions [10]. Therefore, the electrochemistry behind the operation is somewhat different than discussed above.

Anode:

\[
H_2 + CO_2^- \rightarrow H_2O + CO_2 + 2e^-
\]

Equation 2-42
Cathode: \[ \frac{1}{2} O_2 + CO_2 + 2e^- \rightarrow CO_3^{2-} \]  

Overall: \[ H_2 + \frac{1}{2} O_2 + CO_{2,\text{cat}} \rightarrow H_2O + CO_{2,\text{an}} \]  

Hydrogen and oxygen still play the role of fuel and oxidant, but note that \( CO_2 \) is required in the cathode. This is required to create the ion which will travel across the electrolyte into the anode. Note that the ion travels from the cathode to the anode. The \( CO_2 \) is provided by means of mixing the anode and cathode exhaust gas into an oxidizer which combusts any remaining hydrogen generating \( H_2O \) and \( CO_2 \) which is then recirculated into the cathode inlet. This has the double-sided effect of providing \( CO_2 \) necessary for the electrochemistry and also preheating inlet air.

### 2.2.2. Solid Oxide Fuel Cell

A solid oxide fuel cell (SOFC) operates at temperatures closer to 1000 °C. The electrolyte is made up of a ceramic material, typically yttria-stabilized zirconia. The electrodes are also made up of ceramic materials due to the high temperature and the need to closely match thermal expansion coefficients of mated materials. At operating temperature, the electrolyte is conducive to \( O^{2-} \) ions \[10\]. The electrochemistry associated with the SOFC is given below

Anode: \[ H_2 + 2e^- \rightarrow H_2O \]  

Cathode: \[ \frac{1}{2} O_2 + 2e^- \rightarrow O^{2-} \]  

Overall: \[ H_2 + \frac{1}{2} O_2 \rightarrow H_2O \]  

The electrochemistry is very similar to many other types of fuel cells except that the traveling ion is \( O^{2-} \) and it travels from the cathode to the anode similar to the MCFC case. Also, extra fuel
in the exhaust is typically combusted in an oxidizer to generate heat which is then used to preheat air and fuel streams. For this work, the SOFC is considered.

### 2.3. Hydrogen Production

Hydrogen, while the most abundant element in the universe, is rarely found on Earth in its diatomic molecular form. It is attached to some other molecule such as oxygen (in water) or carbon (in crude or natural gas). A few methods have been developed to generate hydrogen for industrial applications - these same methods can be used for generating hydrogen for fuel cells as well.

Due to the high temperatures at which HTFCs operate, they are well suited for stationary power applications while low temperature fuel cells are suited for mobile applications since a warming-up period is not necessary. An HTFC with a megawatt capacity can take several hours to warm up before it reaches temperature and can supply a constant current. As a result, stationary HTFCs usually provide a base load power generation source and are rarely shutdown. It is much more convenient to supply the system with a methane-rich gas (e.g., natural gas, biogas, syngas, etc.) than with pure hydrogen which is energy intensive to produce and transport. Extra heat from the HTFC can be used to reform the natural gas (or other variant) in situ into hydrogen which will participate in the electrochemistry. Low fuel utilization allows for extra hydrogen which can then be separated and used in low temperature fuel cells for mobile applications.

The methods discussed in this section are steam-methane reformation (SMR) and the water-gas shift reaction (WGSR). Both of these methods have been used in industry for various reasons to generate hydrogen and utilize very mature technologies. The application of these methods for
HTFCs provide an interesting synergy which can be used to improve system operation. The steam-methane reformation reaction is given by

\[
\text{CH}_4 + \text{H}_2\text{O}_g \rightarrow 3\text{H}_2 + \text{CO} \quad \Delta H = -206 \frac{kJ}{mol} \quad \text{Equation 2-48}
\]

Where \(\Delta H\) is the change in enthalpy for the reaction. The negative value indicates that the reaction is endothermic meaning it requires heat input. The water-gas shift reaction is given by

\[
\text{CO} + \text{H}_2\text{O}_g \rightarrow \text{CO}_2 + \text{H}_2 \quad \Delta H = 41 \frac{kJ}{mol} \quad \text{Equation 2-49}
\]

It is slightly exothermic meaning it releases heat. Steam-methane reactors typically operate between 550 °C and 900 °C and require a nickel catalyst bed to improve the rate of the reaction. HTFC electrodes are often made of a nickel ceramic and can have the potential to reform methane directly inside the stack [13]. Similar is true for the WGSR; however it requires lower temperatures, around 300 °C, for optimal performance. The carbon monoxide that is generated from SMR is harmless to HTFCs and can even be used as a fuel, but is poisonous to low temperature fuel cells with precious metal catalyst.

**2.4. Hydrogen Separation**

Molecular hydrogen is often mixed with other species which are undesirable or even poisonous to low temperature fuel cells. Carbon monoxide is a poison to the catalyst layer of a proton exchange membrane fuel cell and other species would act as diluents in an otherwise pure stream of hydrogen. Considering the high energy needed to compress or liquefy hydrogen for mobile applications, the hydrogen should be as pure as possible. Pressure swing adsorption (PSA) is currently the oil industry’s standard method of separating hydrogen for its industrial applications. PSA is also a very mature technology which was developed alongside SMR and
WGSR, but other technologies are in development which are not as readily available for larger systems [14].

A typical PSA system requires a significant amount of energy and works by consecutively pressurizing and depressurizing the gas stream over an adsorbent bed. Several stages of compression occur in four to six cylinders. As the pressure in a cylinder increases, hydrogen adsorbs to the bed while the other gas species are suspended and pushed out during the cycle. The gases are moved to the next cylinder where the cycle repeats itself until the target purity is achieved. PSA technology can attain 99.999% purity hydrogen which is suitable for low temperature fuel cells. Unfortunately this comes at the expense of high energy input and system complexity [15].

2.5. Absorption Chilling

Large stationary electricity generation plants often have significant amounts of excess heat coming out of the system exhaust. Often, significant investment is required to convert that heat to electricity through a bottoming cycle such as a Brayton or Rankine cycle if it is to be recovered at all. Absorption chillers enable the usage of the exhaust heat for generating a cooling capacity which can be exported for local cooling or used within the system to improve efficiency.

The more common type of cooling, known as direct expansion or vapor compression cooling, relies on a compressor which is often driven by an electric motor. This compressor compresses a refrigerant fluid, raising its temperature before it goes into a condenser where it rejects heat into the environment. The fluid is then expanded through an expansion valve which lowers its boiling point; it is then passed into an evaporator where it vaporizes. The heat required for vaporization of the fluid results in a drop in temperature in the refrigerant which provides a usable cooling
effect. The fluid then passes to the compressor and the cycle begins anew. A diagram for a direct expansion chiller is shown in Figure 2.

Absorption chillers work on a similar principle as the direct expansion chiller except that the compressor is substituted with a generator and an absorber. Instead of electricity input, absorption chillers require a heat source from an exhaust stream at an elevated temperature. There are two working fluids in this type of chiller, an absorbent and a refrigerant. Similar to the direct expansion chiller, the refrigerant serves the same purpose throughout the cycle in the condenser, expansion valve, and evaporator. The difference lies in the generator and absorber. The refrigerant is absorbed by the absorbent in the absorber into a refrigerant-absorbent solution. This solution is then pumped to a higher pressure into the generator where the heat is introduced. The heat then evaporates the refrigerant and it continues through the cycle first through the evaporator. Remaining absorbent collects back in the absorber and this part of the cycle continues. The diagram for a single-effect absorption cycle is given in Figure 3. The coefficient of performance (COP) of a given chiller is described as
\[ \text{COP} = \frac{Q_c}{W_{in}} \]  \hspace{1cm} \text{Equation 2-50}

Where \( Q_c \) is the cooling load and \( W_{in} \) is the work input. A COP is used instead of efficiency since the amount of cooling can be greater than one. An absorption chiller’s COP is given by

\[ \text{COP} = \frac{Q_c}{Q_{in}} \]  \hspace{1cm} \text{Equation 2-51}

where \( Q_{in} \) is the amount of heat flowing into the generator. The COP of a typical direct expansion chiller can be between four and six whereas the COP of a single-effect absorption chiller is a little less than one.

![Figure 3: Single-effect absorption chiller cycle [16]](image)

Double effect absorption chillers have COPs closer to 1.4 and this increase in efficiency is due to better heat recovery of the exhaust heat stream. A diagram is given below in Figure 4. Vaporized refrigerant from the first generator carries enough heat to vaporize additional refrigerant in the second generator which operates at a lower temperature. Various configurations of heat exchangers exist for this style of absorption chiller, but they all act to recover as much heat as possible within the system so that as much heat as possible is utilized. While the COP of
absorption chillers is lower than that of direct expansion chillers, they cut out the need for a significant electrical load while also enabling the use of exhaust heat which may otherwise go to waste.

Figure 4: Double effect absorption chiller cycle [16]

2.6. Polygeneration using Fuel Cells

High temperature fuel cells generate electricity and useful heat. The electricity is generated at relatively high efficiency compared to other heat engines. Research has been done to look into useful ways to utilize the waste heat from the fuel cell. Some of these methods include electricity generating bottoming cycles, for example, which use gas turbines. Absorption chiller integration has also been a topic of research as well as utilizing the heat for nearby industrial processes [17]–[19].
2.6.1. Tri-Generation

Utilizing heat for the reformation of extra fuel as a result of low fuel utilization combined with hydrogen separation technology has been termed Tri-Generation. The three products are electricity, hydrogen, and heat. Even after hydrogen is produced, there is enough heat exhausting the system to drive a bottoming cycle or to provide heat to an industrial process. A synergy exists within this type of system. A fuel cell operating with low fuel utilization increases the voltage for a given current density (according to Equation 2-27 – the Nernst equation), which in turn, allows for increased efficiency of electricity generation. Additionally, the extra fuel being reformed via SMR requires added heat input. This has the effect of cooling down the stack and as a result, less air needs to be fed into the system which reduces parasitic losses from the air blowers. It has been predicted that a tri-generating HTFC can achieve greater supply chain efficiency of hydrogen production than a centralized SMR plant along with competitive hydrogen prices; this combined with high efficiency electricity generation makes Tri-Generation an attractive option for distributed power and hydrogen generation [6], [20], [7].

A challenge that is present in a tri-generating system is the integration with the PSA system. The exit temperature of an HTFC is very high and the pressure is typically atmospheric. The inlet conditions of the PSA require a temperature of about 25 °C at a pressure of 10 atm. The need to convert a high temperature, low pressure stream to a low temperature, high pressure stream is energy intensive and detracts from the overall system efficiency. The integration of an absorption chiller may be a way to facilitate the temperature change in an efficient manner.
2.6.2. Quad-Generation

Quad-Generation as defined herein is the addition of a separate cooling product to a Tri-Generation system. HTFCs integrated with absorption chillers have been a topic of research and development primarily due to the desire to make fuel cells more appealing to distributed generation schemes.

Systems that integrate a fuel cell and an absorption chiller have been proposed as early as 1992 [21]. Various studies of absorption chillers integrated with HTFCs have shown that the pairing is feasible along with demonstration projects which are currently underway [19], [22]. Certain challenges do exist when devising a CCHP plant that uses fuel cells and absorption chillers. These challenges arise because absorption chillers are typically engineered to require specific inlet conditions that may not match the exhaust conditions of a fuel cell. Margalef et al. studied the impacts of various methods for matching HTFC exhaust to the required inlet conditions of the chiller [18]. For that study, the molten carbonate fuel cell had a high temperature exhaust and a low flow rate compared to the optimal inlet conditions of the chiller. The exhaust was cooled by either mixing ambient air or chiller exhaust; each method presented different impacts on system efficiency where mixing chiller exhaust with fuel cell exhaust was found to be more advantageous.

Other considerations are the availability of direct exhaust fired absorption chillers at a given capacity. Many chillers on the market today are designed to be fired directly from a natural gas furnace or from steam. Not every chiller is fitted with the capability to be exhaust fired partly due to concerns with materials within the heat exchanges that power the generator as well as difficulties that may arise from a variable source of heat. Crystallization of the lithium-bromide solution in absorption chillers is a significant issue that can impact a chiller’s performance and
maintenance schedule. A heat source that is variable complicates the controls designed to avoid crystallization. This is an issue that exists not only with fuel cell and chiller integration, but with any heat source such as gas turbines [23].

Mature technology to separate molecular hydrogen from a gaseous stream exists along with newer technologies that are undergoing research and development. The mature technology is pressure swing adsorption which is utilized heavily in the petroleum industry and was originally patented in 1960 [24], [25]. A typical PSA system requires a significant amount of energy and works by consecutively pressurizing and depressurizing the gas stream over an adsorbent bed. Several stages of compression occur in four to six cylinders. As the pressure in a cylinder increases, hydrogen adsorbs to the bed while the other gas species are suspended and pushed out during the cycle. The gases are moved to the next cylinder where the cycle repeats itself until the target purity is achieved. PSA technology can attain 99.999% purity hydrogen which is suitable for low temperature fuel cells. Unfortunately this comes at the expense of high energy input and system complexity [15].

Newer separation technologies attempt to overcome the challenges of complexity regarding PSA systems and their high energy requirements. Porous membrane technology is one such technology which allows only smaller hydrogen molecules pass through a membrane preventing other species from traversing the membrane. This technology relies on a pressure difference and does not require complex timing of valves and multiple compressors [26]. Electrochemical separation using a proton-conducting membrane is another newer technology which is currently undergoing active research and development. This technology works by using an electrolysis cell by applying a direct current to the membrane which enables hydrogen protons to traverse the membrane selectively. This technology requires a constant power input for a given flux and also,
currently, requires precious metals [14], [20]. For this work, the mature pressure swing adsorption technology is considered.

Hydrogen production using an HTFC has been considered in depth in the past and has led to a number of patents [27]–[29]. The patents illustrate the methodology of utilizing hydrogen generated in the anode for various uses including anode recycling, coal gasification, and purification. Depending on the type of HTFC, there are some system changes that need to be made in order to be able to extract the hydrogen for purification instead of burning it or recycling it through the anode. Specifically, a system which prepares the anode exhaust for separation is required to meet the inlet conditions of a specific separator. For a PSA, this usually requires low temperature and high pressure [15]. Subtle differences exist between operating an MCFC and an SOFC in this mode. For example, an MCFC requires $CO_2$ in the cathode which can either be provided by the anode exhaust or from an oxidizer. The SOFC has no such requirement, so the balance of plant between the two must be different to account for this. The current work only considers SOFCs, so the balance of plant only recirculates exhaust to provide steam to drive the internal steam reformation.

2.7. Summary

A comprehensive study to combine fuel cell technology with hydrogen generation and cooling production has not been found in the literature at this time. In order to better understand the potential methods to improve fuel cell system efficiency as well as to reduce emissions, this work is justified. The current work aims to determine whether the possibility exists to combine the various technologies in a synergistic fashion that ultimately improves system efficiency and provides cooling as a product in addition to electricity, hydrogen, and heat.
3. **APPROACH**

The following tasks were developed which are intended to fulfill the objectives from section 1.3.

1. *Create an integrated computer model of individual components of a baseline Tri-Generation system.*

   A baseline Tri-Generation system will be built as a system to compare against the other models. This system will include an HTFC, reformers, PSA, and other various components such as heat exchangers and blowers. The modeling tool Aspen Plus includes the heat exchangers, blowers, and reformers. Previous work has been done to model the HTFC in FORTRAN and will be integrated into this baseline model.

2. *Create an integrated computer model of individual components of a Quad-Generation system based on the baseline Tri-Generation system.*

   The important operating characteristics of the main components of a Quad-Generation system are the HTFC, absorption chiller, reformers, PSA, and various components such as heat exchangers and blowers. The modeling tool Aspen Plus has the heat exchangers, blowers, and reformers in its library. Previous work has been done to model the HTFC and the chiller in Aspen Plus. Some calculations for the absorption chiller will be done using Microsoft Excel.

3. *Produce a steady-state model of the Quad-Generation system.*

   The individual components of the system must be integrated in such a way that it resembles a real system. Inlet and outlet temperatures and flows of all of the components must be within acceptable bounds defined by manufacturers of similar equipment. The
model will then run until it reaches steady state equilibrium for the given input parameters.

4. Verify that the results of the model match expected results.

The model output is determined by underlying principles included in the library blocks as well as user-generated blocks (e.g., the fuel cell). It also depends on parameters specified for operation. Therefore, the results must be verified to determine that the model is as accurate as possible for the given parameters.

5. Determine the system configuration which optimizes electrical power and hydrogen production efficiency.

Various system configurations are possible each of which has its advantages and disadvantages. The chiller can be utilized to improve Tri-Generating efficiency by providing cooling for the PSA. This configuration will be compared with an electric chiller to determine the most efficient method of cooling down the PSA inlet stream.

6. Determine the system configuration which optimizes electrical power, hydrogen production, and cooling output.

Ideally, the Quad-Generation system will be able to supply the four products to a nearby building or grid. It must be able to do so economically, so in order to increase the economic viability, each of the products must be maximized for any given operating condition. Ultimately, this will depend on the load profile of a given product, but the system configuration will have a large impact on the ability to do so.

7. Implement the models with varying parameters in order to characterize performance.

Three models will be developed, a baseline Tri-Generation model, a Tri-Generation model with an HSU supplemented with an absorption chiller, and a Quad-Generation
model. Each of these models will be run several times with varying parameters such as fuel utilization and power capacity. These results will be used to quantify the performance characteristics of the different systems and apply appropriate comparisons.

4. MODEL DEVELOPMENT

This section will discuss, in detail, the various components and processes that make up the entire system model. The main driver for the model is an SOFC which utilizes the high temperature and water present in the anode to perform internal reformation. Internal reformation as opposed to external reformation is beneficial to SOFC system performance in terms of increased voltage and decreased parasitic cooling loads [15]. The components modeled for the SOFC balance of plant are, the fuel cell itself, a reformer, a pre-reformer, an oxidizer, and several heat exchangers which are used to reuse heat for preheating air and fuel. The main components for the hydrogen separation are water-gas shift reactors, heat exchangers, blowers, and a PSA unit. The absorption chiller is basically made up of various heat exchangers with certain specifications. The integration of these main components is completed with a few more heat exchangers. The modeling platform used for this work is Aspen Plus v7.2. Many of the individual components exist already within the model library of Aspen Plus. The model library does not contain a fuel cell model. However, Aspen Plus does allow for Excel spreadsheets and FORTRAN code to be implemented within the framework of the model as a user generated subsystem. Li et al. built a non-dimensional SOFC model off which this work is based [12]. The absorption chiller model is based off the work of Martz et al [16]. The HSU model is based off the work of Margalef et al. [9].
4.1. SOFC Model

The modeling program Aspen Plus allows for the integration of both pre-existing model library components, user generated components, and calculator blocks that utilize inputs from library components to generate outputs for use elsewhere. The SOFC model uses a combination of these three capabilities. Figure 5 below represents the Aspen Plus SOFC model and the mechanical balance of plant (MBOP).

Fuel comes in at the left and is pressurized, then mixed with a portion of the anode exhaust for preheating and steam addition. The fuel is then preheated to match the inlet temperature of the pre-reformer where it undergoes steam-methane reformation. The stream then enters the SOFC which utilizes FORTRAN code to compute the operating voltage, power, and estimates the exhaust species. The anode exhaust is then sent through an equilibrium reactor which computes the actual species concentration of the stream. That stream is then used to preheat the inlet fuel stream and a portion is sent to the anodic gas oxidizer (AGO). The exhaust of the AGO is used to preheat the incoming air. The air feed is compressed, preheated by the AGO exhaust to the inlet temperature of the SOFC and sent to the SOFC. The exhaust is then sent to the AGO. The below system is based off the work of Margalef for the system integration and Li for the Fortran code which computes energy and electrochemistry [12]. The SOFC model estimates the species concentration based on fuel utilization, but it does not account for the temperature or pressure of the stream. The REFEQ block is used to compute the actual species concentration as a function of the temperature and pressure.
Figure 5: Aspen Plus SOFC model diagram
The SOFC model is capable of producing voltage-current density (V-I) curves which are used for comparison purposes of fuel cell performance. The V-I curves depend entirely upon the Nernst and overvoltage equations presented above. They are listed again below without derivation for convenience:

**Nernst Potential**

\[
V_{\text{Nernst}} = E_0 + \frac{RT}{2F} \ln \left( \frac{p_{H_2}p_{O_2}}{p_{H_2O}} \right)
\]

Equation 4-1

\[E_0\] is calculated by JANAF thermochemical tables[30], [31].

\[E_0 = 1.28628053 - 2.8873 \times 10^{-4} T_{\text{MEA}}\]

Equation 4-2

**Activation Polarization**

\[\eta_{\text{act}} = \eta_{\text{act}}^{\text{an}}(j) + \eta_{\text{act}}^{\text{cat}}(j)\]

\[j = j_0 \left[ \exp \left( \frac{\alpha n F \eta_{\text{act}}}{R_u T} \right) - \exp \left( - \left( 1 - \alpha \right) n F \eta_{\text{act}} \right) \right] \]

Equation 4-3

\[\eta_{\text{act}} = \frac{R_u T_{\text{stack}}}{\alpha n F} \sinh^{-1} \left( \frac{j}{2j_0} \right)\]

Equation 4-4

\[j_{0,\text{an}} = \gamma_\text{an} \left( \frac{p_{H_2}}{p_{\text{amb}}} \right) \left( \frac{p_{H_2O}}{p_{\text{amb}}} \right) \exp \left( - \frac{E_{\text{act,an}}}{R_u T_{\text{stack}}} \right)\]

Equation 4-5

\[j_{0,\text{cat}} = \gamma_{\text{cat}} \left( \frac{p_{O_2}}{p_{\text{amb}}} \right)^{0.25} \exp \left( - \frac{E_{\text{act,cat}}}{R_u T_{\text{stack}}} \right)\]

Equation 4-6

**Ohmic Polarization**

\[\eta_{\text{ohm}} = iR\]

Equation 4-7
\[ \eta_{ohm} = i (R_{an} + R_{elec} + R_{cat} + R_{IC}) \]  
Equation 4-8

\[ R_k = \rho_k \delta_k \]  
Equation 4-9

**Mass Transport or Concentration losses**

\[ \eta_{conc} = c \ln \frac{j_L}{j_L - j} \]  
Equation 4-10

The specific values for the above equations used in the model are given in Table 1 below along with the equations used for computing the ohmic losses of the various components of the MEA [30].

Table 1: Constants used for the electrochemical model

<table>
<thead>
<tr>
<th>Activity Losses</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Anode pre-exponential factor ( \gamma_{an} )</td>
<td>5.5 \times 10^8 , A \cdot m^{-2}</td>
</tr>
<tr>
<td>Anode activation energy ( E_{\text{act,an}} )</td>
<td>50,000 , J \cdot mol^{-1}</td>
</tr>
<tr>
<td>Cathode pre-exponential factor ( \gamma_{cat} )</td>
<td>7 \times 10^8 , A \cdot m^{-2}</td>
</tr>
<tr>
<td>Cathode activation energy ( E_{\text{act,cat}} )</td>
<td>117,000 , J \cdot mol^{-1}</td>
</tr>
</tbody>
</table>

**Ohmic Losses**

<table>
<thead>
<tr>
<th>Component</th>
<th>Expression</th>
</tr>
</thead>
<tbody>
<tr>
<td>Specific resistivity of the anode ( \delta_{an} )</td>
<td>[ \left[ \frac{95 \times 10^6}{T_{\text{stack}}} \exp \left( - \frac{7150}{T_{\text{stack}}} \right) \right]^{-1} , \Omega \cdot m ]</td>
</tr>
<tr>
<td>Specific resistivity of the cathode ( \delta_{cat} )</td>
<td>[ \left[ \frac{42 \times 10^8}{T_{\text{stack}}} \exp \left( - \frac{7200}{T_{\text{stack}}} \right) \right]^{-1} , \Omega \cdot m ]</td>
</tr>
<tr>
<td>Specific resistivity of the electrolyte ( \delta_{ele} )</td>
<td>[ \left[ 3.34 \times 10^4 \exp \left( - \frac{1030}{T_{\text{stack}}} \right) \right]^{-1} , \Omega \cdot m ]</td>
</tr>
<tr>
<td>Specific resistivity of the interconnects ( \delta_{IC} )</td>
<td>[ \left[ \frac{9.3 \times 10^6}{T_{\text{stack}}} \exp \left( - \frac{1100}{T_{\text{stack}}} \right) \right]^{-1} , \Omega \cdot m ]</td>
</tr>
<tr>
<td>Anode thickness ( \delta_{an} )</td>
<td>1 \times 10^{-3} , m</td>
</tr>
</tbody>
</table>
Cathode thickness $\delta_{ca}$ | $5 \times 10^{-5} m$
Electrolyte thickness $\delta_{el}$ | $1 \times 10^{-5} m$

**Concentration Losses**

- Pre-multiplication constant $c$ | 0.05
- Limiting current density $j_L$ | $10,001 A \cdot m^{-2}$

### 4.2. Hydrogen Separation Unit

The Tri-generation of electricity, hydrogen, and heat depends on equipment that is installed downstream of the anode exhaust. Two water-gas shift reactors which operate at a high and low temperature are used to react any remaining carbon monoxide to create as much hydrogen as possible. The water-gas shift reaction is repeated below:

$$CO + H_2O_g \rightarrow CO_2 + H_2 \quad \text{Equation 4-11}$$

The high temperature reactor operates at 300 °C and takes advantage of faster kinetics to quickly shift the $CO$ to $H_2$. The low temperature operates at 200 °C and is able to shift more $CO$ to increase the overall $H_2$ concentration [32]. After the shift reactors, the stream is hydrogen rich and must be cooled before entering the PSA. Due to the high pressure target, a two stage compression is modeled with cooling in between. Water is condensed out of the stream through flash blocks to ensure that the stream has a vapor fraction of one as it enters the compressors. Finally, water chilled from an electric chiller is used to cool the hydrogen rich stream to the required inlet temperature of the PSA at 25 °C. The air used for intercooling is mixed and later pre-heated for the cathode inlet. The diagram of the HSU is presented in Figure 6 below.
Figure 6: Hydrogen separation unit system diagram
4.3. Absorption Chiller Model

A double-effect absorption chiller model was utilized for this work to investigate integration with the system. The chiller, like the fuel cell system, was modeled in Aspen Plus and takes advantage of Aspen’s model library. The fuel cell exhaust is fed into the first generator and then through a solution heat exchanger where it exhausts out of the system entirely. The model is based off Martz’s work and is tuned to emulate the Yazaki CH-KE-4040 chiller which is designed to provide about 140 kW of cooling to a chilled water loop. It is basically made up of a series of heat exchangers and other components placed inside hierarchies which represent the main components of the absorption chiller (generators, condenser, evaporator, absorber, and solution heat exchangers). The chiller model is scalable to larger sizes, though some issues begin to impact results at larger sizes. The chiller design diagram from Figure 4 is copied below for convenience as that is the same system which is modeled by Martz [16]. Two methods of ensuring that the inlet temperature of the chiller is maintained to specification are used. One is to mix the inlet stream with ambient air to obtain a specific temperature. The other is to use recirculate a portion of the chiller exhaust and mix it with the inlet stream. The second method has lower change in temperature between the two streams, so there is less entropy generation as a result. The second approach results in higher efficiency operation with a fuel cell [18].
A single effect absorption chiller model was also developed from the above model to investigate the Tri-Generation system configuration. The main difference is that the second generator is removed and only a single heat exchanger exists between the generator and the absorber (see Figure 3).

4.4. System Configuration Models

One objective is to investigate the effectiveness of integrating an absorption chiller within the system to improve Tri-Generation performance. Another objective of this work is to combine the above models and quantify the system performance for comparison with other means of generating the desired products (electricity, cooling, heat, and hydrogen).
4.5. Tri-Generation Model

A guide for modeling a Tri-Generation model was developed by the National Renewable Energy Laboratory which gives specific guidance for an MCFC system [33], [34]. The current work is relying on SOFC technology, nevertheless, the modeling principles are similar. The HSU is placed as a hierarchy block in the anode exhaust stream after it has been recirculated to preheat the incoming fuel. A portion of the anode exhaust is mixed with the fuel in order to mix the resident steam with fuel for the steam-methane reaction. A design specification is set to ensure that a specific steam-to-carbon ratio is maintained. Equation 2-48 is the SMR reaction and the stoichiometry requires only a ratio of unity. However, under certain conditions, coking can occur at low ratios therefore a steam-to-carbon ratio of about three yields the fastest rate [35].

The anode exhaust stream enters the HSU at a temperature much higher than the operating temperature of the high-temperature shift reactor. Air is used to cool the anode exhaust to 300 °C for use in the shift reactor and that heated air is used for the cathode inlet. The stream is cooled again to accommodate the inlet conditions for the low temperature reactor (200 °C). Air cooling is used again after the reactor in preparation for two-stage compression. Water is then used to cool the stream to accommodate the PSA inlet conditions. A percentage of the air used for cooling inside the HSU is further heated by the oxidizer exhaust then sent to the cathode. The amount sent into the cathode is determined by a design spec with the following formula built in

\[ \dot{n}_{\text{air}} = \frac{n_{\text{fuelin}}(q_{FP} + 4U_F(\Delta h_f + n_eF(-0.28U_f^2 + 0.15U_f + 0.77)))}{c_p(T)\Delta T} \]

where \( \dot{n} \) is the molar flow either air or fuel, \( q_{FP} \) is the specific heat absorbed by the fuel processing reactions, \( U_F \) is the fuel utilization, \( n_e \) is the number of electrons that participate in the reaction, \( F \) is Faraday’s constant, \( c_p(T) \) is the specific heat of air, and \( \Delta T \) is the temperature.
increase between the inlet and exit of the fuel cell. The derivation of Equation 4-12 is discussed in Margalef’s dissertation work [9]. The Aspen system diagram is presented in Figure 8 below.

The inlet conditions of the PSA require a high pressure stream of 10 atmospheres at a temperature of 25 °C. The anode exhaust conditions are typically at a high temperature and low pressure. As a result, a two stage compression system with intercooling from ambient air and an electric chiller is typically used to meet the inlet conditions of the PSA. An absorption chiller is capable of providing enough cooling to the stream by using the heat available within the stream itself. This has the advantage of cutting out the electric chiller and reducing parasitic loads. To achieve this configuration, the absorption chiller is placed directly in the anode exhaust following the low temperature WGSR after a single compressor; as the pressure is increased the temperature increases according to the ideal gas law. The stream must then be cooled to meet the inlet temperature requirement of the absorption chiller. Cooling water is produced at 7 °C which is then used to cool the pressurized anode exhaust to the required 25 °C through a heat exchanger. There is enough leftover cooling available to cool the anode exhaust after the low temperature WGSR prior to compression. For a megawatt scale system, the mass flow of the anode exhaust is not enough to support the operation of a double effect absorption chiller. As a result, a single effect absorption chiller must be used. The HSU configuration is presented in Figure 9 below. The configuration described above is compared to a configuration that utilizes an electric chiller to cool the stream prior to the PSA inlet after a two-stage compression with intercooling configuration.
Figure 8: Tri-Generation system diagram
Figure 9: Tri-generation and absorption chiller integration within the HSU
4.6. Quad-Generation Model

To meet the Quad-Generation objective, the HSU is placed downstream of the anode exhaust and the absorption chiller is placed downstream of the system exhaust. An analysis of the heat flow of various streams identified the system exhaust as the most advantageous location for the chiller to maximize cooling potential. This is a result of the high mass flow and the temperature of the exhaust compared to the other system streams. Also, for system integration, this poses the easiest location as it does not impact any downstream components.

In order to determine the optimal location for the absorption chiller, an analysis of each stream was conducted to understand the thermodynamic properties which are important to the integration of a chiller. These properties were used in order to determine where the highest quality of heat was available within the whole system. The two main properties for the analysis were the stream temperature and the flow rate. In order to match the inlet specifications of the chiller, a stream had to have a temperature greater than or equal to 280 °C with a flow rate that is sufficient for a given size. Care was also taken to avoid streams that required a specific temperature or mass flow for proper operation. For example, the cathode inlet stream was calculated to be 900 °C with a relatively high flow rate; however, deviation from the specified temperature or flow rate would impair the fuel cell’s performance. One location that was seriously considered was the oxidizer exhaust stream. The temperature of that stream was calculated to about 1200 °C. A significant amount of heat was available from that stream to be used for a chiller. In reality, any removal of heat from that stream took away that much available preheat for the fuel and air inlet streams. Therefore, only a small amount of heat could be extracted – not enough to be considered worthwhile. The cathode exhaust prior to the oxidizer
was considered as well, but this affected the performance of the oxidizer. It also didn’t have as high of a flow rate compared to the system exhaust, so not as much cooling was available. This type of analysis was done for each stream and ultimately, the system exhaust proved to be able to meet the required thermodynamic properties and it didn’t have any impact on any downstream system operation. This is also what ultimately led to the discovery of the location for a chiller in the hydrogen booster even though that location did not provide any cooling as an additional product.

To meet the inlet temperature requirement of the absorption chiller, a design specification is used in the HSU which controls the air flow used for system cooling. This specification is set to watch the exhaust temperature and adjust the air flow to ensure a temperature of 280 °C enters the absorption chiller. A separate design specification is used to solve for Equation 4-12 which controls a stream splitter ensuring that the appropriate amount of air is used for cooling the stack. The system configuration is presented in Figure 10 below.
Figure 10: Quad-Generation system diagram
4.7. Efficiency Calculations

In order to determine the efficiency of a tri-generating system a few methods have been developed by Margalef et al. [36]. For the purposes of this work, the Supplemental Inputs Method is used for Tri-Generation efficiency calculations. The equations for the Supplemental Inputs Method are below:

\[
\eta_{\text{electric}} = \frac{P_{\text{net}}}{E_{\text{tot}} \left( \frac{Q_e}{\eta_{\text{boiler}}} \right) - \left( U_F - U_{F,H2ES} \right) E_{\text{tot}} + \frac{P_{\text{PSA}}}{\eta_{\text{CC}}}} \quad \text{Equation 4-13}
\]

\[
\eta_{\text{thermal}} = \eta_{\text{boiler}} \quad \text{Equation 4-14}
\]

\[
\eta_{H_2} = \frac{H}{\left( U_F - U_{F,H2ES} \right) E_{\text{tot}} + \frac{P_{\text{PSA}}}{\eta_{\text{CC}}}} \quad \text{Equation 4-15}
\]

\[
\eta_{\text{total}} = \frac{P_{\text{net}} + Q_{\text{net}} + H}{E_{\text{tot}}} \quad \text{Equation 4-16}
\]

Where \(P_{\text{net}}\) is the net electric power produced, which is given by subtracting the balance of plant power usage from the gross power generated by the fuel cell. \(E_{\text{tot}}\) is the total energy input into the system, \(Q_e\) is the heat associated with electricity production, \(\eta_{\text{boiler}}\) is the efficiency of the heat recovery system, \(U_F\) is the normal fuel utilization of a typical HTFC, \(U_{F,H2ES}\) is the fuel utilization when hydrogen is produced, \(P_{\text{PSA}}\) is the power used by the PSA system, \(\eta_{\text{CC}}\) is the hydrogen separation efficiency, \(H\) is the total energy of the hydrogen product, and \(Q_{\text{net}}\) is the total recoverable heat.
When cooling is introduced as an additional product, the efficiency calculation becomes more complicated. This is due to how refrigeration cycles are characterized in terms of efficiency. The COP (as described in Equation 2-51) is used as a factor for comparing the efficiency of various refrigeration cycles. Since the amount of cooling energy supplied by an absorption chiller can be greater than the amount of heat provided, the overall system efficiency can be greatly exaggerated if cooling energy is simply added to the numerator of the total efficiency calculation:

\[
\eta_{\text{total}} = \frac{P_{\text{net}} + Q_{\text{net}} + H + Q_c}{E_{\text{tot}}} \quad \text{Equation 4-17}
\]

An alternative approach is to consider the heat recovery of the absorption chiller instead of the cooling product. The amount of heat recovered from the exhaust stream for use in the chilling cycle may be used as an input in the efficiency calculation.

\[
\eta_{\text{total}} = \frac{P_{\text{net}} + Q_{\text{net}} + H + (Q_{\text{exh}} - Q_{\text{exh,c}})}{E_{\text{tot}}} \quad \text{Equation 4-18}
\]

where \(Q_{\text{exh}}\) is the heat of the exhaust stream entering the chiller’s generator and \(Q_{\text{exh,c}}\) is the heat of the exhaust exiting the chiller.
5. RESULTS

5.1. Model Verification

In order to verify the model performance, the same approach developed by Mu Li for his dissertation work and used by Pere Margalef for his dissertation work is appropriate for this work since a similar electrochemical model is used. Li based his approach on the IEA Benchmark which is a result of modeling efforts conducted by several nations in Europe and Japan. The benchmark was developed under specific operating parameters of a single button cell for two different cases. Two cases are listed below in Table 2. Benchmark 1 refers to the case for humidified hydrogen and Benchmark 2 refers to the case of a methane and hydrogen mixture. For this work, only Benchmark 2 is used.

Table 2: IEA Benchmark operating parameters

<table>
<thead>
<tr>
<th>System Pressure</th>
<th>100 kPa</th>
</tr>
</thead>
<tbody>
<tr>
<td>Periphery conditions</td>
<td>Adiabatic</td>
</tr>
<tr>
<td>Inlet Fuel and Air Temperature</td>
<td>1173K</td>
</tr>
<tr>
<td>Air utilization (O\textsubscript{2} basis)</td>
<td>14%</td>
</tr>
<tr>
<td>Fuel Utilization</td>
<td>85%</td>
</tr>
<tr>
<td>Mean current density</td>
<td>3000 A/m\textsuperscript{2}</td>
</tr>
</tbody>
</table>
| Inlet gas composition (Benchmark 1) | Fuel: 90% H\textsubscript{2}; 10% H\textsubscript{2}O (mole basis) 
Air: 21% O\textsubscript{2}; 79% N\textsubscript{2} (mole basis) |
| Inlet gas composition (Benchmark 2) | Fuel: 26.26% H\textsubscript{2}, 17.1% CH\textsubscript{4}, 2.94% CO, 4.36% CO\textsubscript{2}, 49.34% H\textsubscript{2}O (mole basis)  
Air: 21% O\textsubscript{2}; 79% N\textsubscript{2} (mole basis) |
Figure 11: 1 atm IEA benchmark comparison

Figure 12: 2 atm IEA benchmark comparison
The comparison that Margalef performed yielded results which indicated that their model best predicts results for the 1 atm case [9]. The current model’s trend matches well with the benchmark, but it predicts a low voltage for each pressure case. Without correcting for the low prediction, the percent error between the current model and the IEA benchmark results hovers around 10%. If the voltage is corrected by subtracting the difference between the first point and the associated point from the model results, the percent error is no greater than 2% for any case.

A comparison was also made with work done by Jiang and Virkar in order to compare the model against experimental results [37]. Their experimental work focused on various anode gas concentrations.
The model follows a similar trend to the experimental results. With the difference between the two subtracted, the following results give relative errors no greater than 2.20%. These results suggest that the JANAF thermochemical table (Equation 4-2) doesn’t agree with Jiang and Virkar’s experimental results or the IEA benchmark [37]. However, the model does follow the trend very closely for both the experimental results and the IEA benchmark.

Figure 14: Experimental results and model comparison
5.2. Baseline Tri-Generation Model Results

In order to appropriately compare the different system configurations, the model was implemented using a configuration for a baseline Tri-Generation system. Namely, the changes in power and efficiency will be compared; changes in hydrogen production will be discussed as well. The operating current density was 7000 A/m². The efficiency was calculated using the Supplemental Inputs Method as described by Equation 4-16.

Figure 16 presents the nominal power produced by the fuel cell as a function of the different fuel utilizations. The trend is common between all of the specified power cases due to the bulk modeling approach. More power is produced as the fuel utilization is increased since more fuel is undergoing electrochemical reactions. This, in turn, generates more heat which requires greater cooling from the balance of plant.
Figure 16: Change in the nominal power and BOP power of a baseline 1 MW Tri-Generation system as a function of fuel utilization.
Figure 17 presents the BOP parasitic subtracted from the nominal power resulting in the net power which is available as a product outside the system.

![Net Power (1 MW) Diagram](image1)

**Figure 17: Change in the net of a baseline 1 MW Tri-Generation system as a function of fuel utilization**

![Electrical Efficiency (1 MW) Diagram](image2)

**Figure 18: Electrical efficiency calculation method for a 1 MW baseline Tri-Generation system**

The Supplemental Inputs Method is useful for a polygenerating system since all energy input is not dedicated to a single product, this allows for a more meaningful efficiency comparison.
between systems [36]. Figure 18 presents the electrical efficiency of the system as a function of fuel utilization. Both the Supplemental Inputs Method and the common net energy divided by energy input method are presented. The effect of increasing fuel utilization on electrical efficiency is clear. At fuel utilizations greater than 0.65, the Supplemental Inputs Method efficiency calculations are less than the traditional power divided by energy input. This is a result of less energy being available to the other valuable products and without the added benefit to the electrical efficiency at higher utilizations.

The calculated hydrogen flow is presented in Figure 19. Predictably, the available hydrogen decreases as fuel utilization increases. This is due to less available hydrogen in the anode exhaust being sent to the WGSR.

![Hydrogen Flow (1 MW)](image)

Figure 19: Change in hydrogen mass flow as a function of fuel utilization of a baseline 1 MW Tri-Generation system

The hydrogen output varies linearly as a function of fuel utilization. This is due to the direct impact of the fuel utilization on the amount of available hydrogen in the anode exhaust stream. Higher fuel utilization means that more fuel is consumed due to electrochemical reactions which results in less exhausted hydrogen.
Figure 20 presents the computed useful heat exiting the system. This calculation assumes a 100 °C drop in exhaust temperature and 90% efficient heat recovery. Figure 21 presents the system exhaust temperature variation. The same assumption is used for the total efficiency calculation in Figure 22.

Figure 20: Change in useful heat as a function of fuel utilization of a baseline 1 MW Tri-Generation system

Figure 21: Change in exhaust temperature of a 1 MW baseline Tri-Generation system
Figure 22 presents the total system efficiency of the baseline 1 MW Tri-Generation system. The total efficiency accounts for power, hydrogen, and heat recovery.

![Figure 22: Product efficiencies of a 1 MW baseline Tri-Generation system](image)

Table 3 and Table 4 present results from various cases run at different nominal power ratings for 0.6 and 0.85 fuel utilization respectively. The average calculated efficiency for the baseline Tri-Generation system is 92.2% given a 100 °C drop in exhaust temperature for heat recovery and fuel utilization of 0.6. For a fuel utilization of 0.85, the average efficiency is 74.5%. The large difference in efficiency is a direct result of the impacts of the fuel utilization has on the product various products. A lower utilization enables a higher cell voltage which directly correlates to higher electrical efficiency. Furthermore, the lower utilization allows for more hydrogen to be produced. In each case, the PSA uses the same parasitic for a given power capacity, but does not vary with fuel utilization. As a result, the PSA has a larger impact on the system efficiency when less hydrogen is being produced.

55
The nominal power was varied by adjusting the initial fuel flow. As a rule of thumb, an increase of 7 kmol/hr of fuel correlated to about a megawatt of nominal fuel cell power. While the amounts of products were expected to increase with increased nominal power, the system efficiency was expected to remain the same given that the model is a bulk model. The results show that while the efficiency doesn’t deviate by more than a couple percentage points, it does vary, but without a noticeable correlation to the power rating. The reason for this variation is not fully understood. Upon closer inspection, the hydrogen flow does not follow a strictly linear correlation to power as the power and heat products. This indicates that a component within the hydrogen booster is sensitive to varying flow rates that result from the different nominal power ratings. This phenomenon is not enough to vary the efficiency in a significant manner.
Table 3: Product results and total system efficiency for a 1 MW Tri-Generation system at 0.6 fuel utilization

<table>
<thead>
<tr>
<th>Nominal Power (MW)</th>
<th>Net Power (kW)</th>
<th>Hydrogen Flow (kg/hr)</th>
<th>Heat (kW)</th>
<th>System Efficiency (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>829.3</td>
<td>11.7</td>
<td>843.8</td>
<td>92.0%</td>
</tr>
<tr>
<td>2</td>
<td>1,694.9</td>
<td>22.4</td>
<td>1,694.9</td>
<td>92.0%</td>
</tr>
<tr>
<td>3</td>
<td>2,607.8</td>
<td>30.9</td>
<td>2,607.8</td>
<td>94.0%</td>
</tr>
<tr>
<td>4</td>
<td>3,457.1</td>
<td>40.6</td>
<td>3,457.1</td>
<td>91.9%</td>
</tr>
<tr>
<td>5</td>
<td>4,197.1</td>
<td>58.6</td>
<td>4,197.1</td>
<td>92.3%</td>
</tr>
<tr>
<td>6</td>
<td>5,187.4</td>
<td>60.7</td>
<td>5,187.4</td>
<td>91.8%</td>
</tr>
<tr>
<td>7</td>
<td>5,879.3</td>
<td>81.7</td>
<td>5,879.3</td>
<td>92.3%</td>
</tr>
<tr>
<td>8</td>
<td>6,908.2</td>
<td>81.6</td>
<td>6,908.2</td>
<td>91.9%</td>
</tr>
<tr>
<td>9</td>
<td>7,622.8</td>
<td>101.4</td>
<td>7,622.8</td>
<td>92.2%</td>
</tr>
<tr>
<td>10</td>
<td>8,470.4</td>
<td>112.7</td>
<td>8,470.4</td>
<td>92.1%</td>
</tr>
</tbody>
</table>
Table 4: Product results and total system efficiency for a 1 MW Tri-Generation system at 0.85 fuel utilization

<table>
<thead>
<tr>
<th>Nominal Power (MW)</th>
<th>Net Power (kW)</th>
<th>Hydrogen Flow (kg/hr)</th>
<th>Heat (kW)</th>
<th>System Efficiency (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>609.0</td>
<td>3.6</td>
<td>432.8</td>
<td>74.4%</td>
</tr>
<tr>
<td>2</td>
<td>1224.3</td>
<td>7.0</td>
<td>865.5</td>
<td>74.5%</td>
</tr>
<tr>
<td>3</td>
<td>1851.6</td>
<td>10.1</td>
<td>1298.1</td>
<td>74.5%</td>
</tr>
<tr>
<td>4</td>
<td>2475.6</td>
<td>13.3</td>
<td>1730.8</td>
<td>74.5%</td>
</tr>
<tr>
<td>5</td>
<td>3032.9</td>
<td>18.6</td>
<td>2164.2</td>
<td>74.6%</td>
</tr>
<tr>
<td>6</td>
<td>3603.7</td>
<td>23.4</td>
<td>2597.4</td>
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</tr>
<tr>
<td>7</td>
<td>4250.0</td>
<td>25.9</td>
<td>3029.8</td>
<td>74.6%</td>
</tr>
<tr>
<td>8</td>
<td>4896.2</td>
<td>28.4</td>
<td>3462.1</td>
<td>74.5%</td>
</tr>
<tr>
<td>9</td>
<td>5509.1</td>
<td>31.9</td>
<td>3894.9</td>
<td>74.6%</td>
</tr>
<tr>
<td>10</td>
<td>6121.6</td>
<td>35.5</td>
<td>4327.7</td>
<td>74.6%</td>
</tr>
</tbody>
</table>
Figure 23: Efficiency comparison of baseline Tri-Generation system as a function of power

5.3. Quad-Generation Model Results

The fuel cell electrochemical model combined with the balance of plant model and a double effect absorption chiller was used to run several cases of varying parameters. Most notably, for a nominal 150 kW system and a 1 MW system, the fuel utilization was varied in order to determine the impact on the power produced, the hydrogen produced, and the cooling produced as well as the efficiency of each product.

The nominal power produced varies as a function of the fuel utilization due to varying levels of fuel being reacted in the stack. Figure 24 and Figure 25 present the nominal power available from the 150 kW and 1 MW systems as a function of fuel utilization. Also plotted is the change in BOP power requirements. More power can be generated when more fuel is allowed to electrochemically react. This directly affects the balance of plant and requires greater parasitic losses as a result of the greater heat generated at higher fuel utilizations.
The net power produced varies as a function of the fuel utilization due to changes in the electrochemistry which also alters the balance of plant requirements. Net power for the 150 kW and the 1 MW cases are plotted in Figure 26 and Figure 27.
The trends in many of these plots will appear similar when comparing sizes; this is due to the bulk model operating at steady state. It is interesting to point out that there is a wide range for the net power for a constant fuel flow rate. This is partly due to when the fuel utilization is increased the fuel concentration in the exit of the anode is reduced, thus reducing the Nernst potential. This
impact directly affects the operating voltage of the fuel cell which in part determines the electrical efficiency. Furthermore, the use of internal steam-methane reformation provides additional cooling benefit to the system without additional balance of plant input. As a result, the system can provide more power with lower parasitic loads. This effect is evident in the electrical efficiency calculations.

Since many trends will be similar between the 150 kW and the 1 MW size, the following hydrogen results will be normalized by the power. So, for example, Figure 28 presents the product hydrogen flow divided by the nominal power output of the system. The actual amount of hydrogen varies depending on the size, but the trend as a function of fuel utilization remains roughly the same. As is evident, the amount of available hydrogen decreases as fuel utilization increases. A slightly larger decrease between 0.6 and 0.65 is observed than for the rest of the points. The general trend is due to less hydrogen available in the anode tail gas for the hydrogen booster to recuperate and separate.

![Normalized Hydrogen Flow (150 kW - 1 MW)](image)

Figure 28: Normalized variance of hydrogen as a function of fuel utilization (150 kW – 1 MW)
The model was also used to simulate systems greater than 2 MW up to 10 MW. The 150 kW and 1 MW systems are mentioned separately since numerical errors began to drastically affect the results of the larger sizes. Most noticeable was the chiller COP which, for the 150 kW system, is expected to fall between 1.1 and 1.4. The larger sizes would produce a COP below 1 for several different parameters. As a result, these cases were modeled separately with the COP acting as an additional parameter. The same trends occurred for these cases as well, but the results are a little different. Results presented will be separated to make clear the distinction between power capacities. Figure 29 presents the normalized hydrogen flow for the 2 MW to 10 MW cases. The amount of hydrogen produced from this system configuration is slightly lower than the case where the actual chiller model is used.

The product results at 0.6 fuel utilization for each size case is presented in Table 5 below. The total system efficiency for the 150 kW and the 1 MW Supplemental Inputs Method was calculated as expressed in Equation 4-18. For the 2 MW to 10 MW sizes, the COP of the chiller was varied from 0.85 to 1.5. Below are the calculated efficiencies at a nominal COP of 1.1 and a
fuel utilization of 0.6. A COP of 1.1 was chosen as the nominal COP since that is what the double-effect chiller consistently computed for its COP at the lower sizes. Above 1 MW, the calculated COP diminished further as the size grew larger. This is not likely to occur in a real system where the COP is often rated above 1.0 and is normally closer to 1.4. With this in mind, the calculated system efficiencies should be somewhat conservative. Table 6 presents the same results except under 0.85 fuel utilization operation.
Table 5: Quad-Generation product results at 0.6 fuel utilization and fixed COP of 1.1

<table>
<thead>
<tr>
<th>Nominal Power (MW)</th>
<th>Net Power (kW)</th>
<th>Hydrogen Flow (kg/hr)</th>
<th>Cooling (kW)</th>
<th>Heat (kW)</th>
<th>System Efficiency (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.150</td>
<td>109</td>
<td>1.51</td>
<td>68.59</td>
<td>7.88</td>
<td>80.0%</td>
</tr>
<tr>
<td>1</td>
<td>811.0</td>
<td>10.6</td>
<td>923.1</td>
<td>116.5</td>
<td>85.0%</td>
</tr>
<tr>
<td>2</td>
<td>1623.9</td>
<td>21.4</td>
<td>1402.3</td>
<td>232.4</td>
<td>84.7%</td>
</tr>
<tr>
<td>3</td>
<td>2470.5</td>
<td>30.4</td>
<td>1844.5</td>
<td>353.0</td>
<td>85.4%</td>
</tr>
<tr>
<td>4</td>
<td>3267.4</td>
<td>42.9</td>
<td>2317.4</td>
<td>464.4</td>
<td>85.3%</td>
</tr>
<tr>
<td>5</td>
<td>4106.2</td>
<td>52.5</td>
<td>2795.3</td>
<td>583.4</td>
<td>85.1%</td>
</tr>
<tr>
<td>6</td>
<td>4950.6</td>
<td>61.7</td>
<td>3260.9</td>
<td>703.7</td>
<td>85.1%</td>
</tr>
<tr>
<td>7</td>
<td>5779.4</td>
<td>72.0</td>
<td>3726.7</td>
<td>820.9</td>
<td>85.1%</td>
</tr>
<tr>
<td>8</td>
<td>6608.2</td>
<td>82.2</td>
<td>4192.5</td>
<td>938.2</td>
<td>85.2%</td>
</tr>
<tr>
<td>9</td>
<td>7436.9</td>
<td>92.5</td>
<td>4658.4</td>
<td>1055.5</td>
<td>85.2%</td>
</tr>
<tr>
<td>10</td>
<td>8265.7</td>
<td>102.8</td>
<td>923.1</td>
<td>1172.8</td>
<td>85.0%</td>
</tr>
</tbody>
</table>

The average system efficiency according to the Supplemental Inputs Method across the different sizes is 84.6%. The average efficiency excluding the 150 kW and the 1 MW case is 85.1%. Table 6 presents the same analysis, except for 0.85 fuel utilization case. The average efficiency is 68.7% and with the 150 kW and the 1 MW excluded, the efficiency is 70.5%.
Table 6: Quad-Generation product results at 0.85 fuel utilization

<table>
<thead>
<tr>
<th>Nominal Power (MW)</th>
<th>Net Power (kW)</th>
<th>Hydrogen Flow (kg/hr)</th>
<th>Cooling (kW)</th>
<th>Heat (kW)</th>
<th>System Efficiency (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>560.1</td>
<td>3.3</td>
<td>1230.3</td>
<td>309.9</td>
<td>70.0%</td>
</tr>
<tr>
<td>2</td>
<td>1122.9</td>
<td>6.7</td>
<td>2460.8</td>
<td>619.8</td>
<td>70.1%</td>
</tr>
<tr>
<td>3</td>
<td>1713.3</td>
<td>9.4</td>
<td>3689.6</td>
<td>929.4</td>
<td>70.3%</td>
</tr>
<tr>
<td>4</td>
<td>2266.0</td>
<td>13.4</td>
<td>4921.7</td>
<td>1239.7</td>
<td>70.5%</td>
</tr>
<tr>
<td>5</td>
<td>2851.2</td>
<td>16.3</td>
<td>6150.3</td>
<td>1549.2</td>
<td>70.5%</td>
</tr>
<tr>
<td>6</td>
<td>3440.0</td>
<td>19.1</td>
<td>7379.3</td>
<td>1858.8</td>
<td>70.6%</td>
</tr>
<tr>
<td>7</td>
<td>4017.0</td>
<td>22.3</td>
<td>8609.2</td>
<td>2168.6</td>
<td>70.6%</td>
</tr>
<tr>
<td>8</td>
<td>4594.0</td>
<td>25.4</td>
<td>9839.1</td>
<td>2478.4</td>
<td>70.6%</td>
</tr>
<tr>
<td>9</td>
<td>5170.9</td>
<td>28.6</td>
<td>11069.0</td>
<td>2788.2</td>
<td>70.6%</td>
</tr>
<tr>
<td>10</td>
<td>5747.9</td>
<td>31.8</td>
<td>12298.8</td>
<td>3098.0</td>
<td>70.7%</td>
</tr>
</tbody>
</table>

Figure 30 presents the efficiency graphs of the product results at 0.6 and 0.85 fuel utilization. The efficiency stays relatively constant for any given power capacity between 1 and 10 megawatts. Figure 31 presents the same results except with a fixed COP of 1.4. With the higher efficiency chiller, the effect of varying fuel utilization on system efficiency diminishes. This result suggests that Quad-Generation with a high efficiency chiller could negate any negative effects on the system level. This would enable flexibility in system operation by allowing for preference of a specific product while maintaining system efficiency.
Figure 30: Total efficiency comparison of a Quad-Generation system as a function of nominal power at 1.1 COP

Figure 31: Total efficiency comparison of a Quad-Generation system as a function of nominal power at 1.4 COP
Figure 32 and Figure 33 present the electric and heat products of the baseline Tri-Generation system and the Quad-Generation system at 10 MW respectively. The trends for the power and heat are similar between the two as well as the approximate values. The available heat is
determined by a 100 °C drop in temperature and a 90% effective heat recovery device. An absorption chiller is capable of extracting more heat as well as multiplying the useful product with a large COP. The impact of this result is that a Quad-Generation system can be operated without varying efficiency given any fuel utilization. This allows for potential dynamic operation for a load that has varying power and cooling demands.

5.4. Supplemented Tri-Generation Model Results

Similar to the Quad-Generation model, the chiller supplemented Tri-Generation model was run under various conditions to quantify its performance characteristics. Figure 34 presents the nominal power and BOP requirements as a function of fuel utilization. The nominal power increases as a function of fuel utilization similar to the Quad-Generation results. The parasitic losses associated with the BOP increase similarly due to the increased cooling requirement. Figure 35 presents the net power available from the chiller supplemented system compared with the baseline system. It follows a similar trend as for the Quad-Generation system. However, comparing the baseline results and the supplemented results, the available net power is different for each utilization factor. At higher utilization, the baseline case has much lower net power available whereas at lower utilizations, the systems offer about the same amount of power. There is a much larger discrepancy between the high utilization and low utilization. It varies from about 850 kW to just over 600 kW. For the chiller-supplemented case, the variation of power is significantly smaller, varying from just under 830 kW to just over 800 kW. This difference is likely due the greater cooling demand in the HSU for the baseline case which uses an electric chiller and will require more energy to cool the anode exhaust going through the HSU. The chiller-supplemented case does not have this parasitic loss, so the increased parasitic is not nearly as pronounced. However, running a fuel cell at high fuel utilization will lead to poor
hydrogen production, so such operation may not be ideal for either Tri-Generation case while hydrogen is desired.

Figure 34: Change in the nominal power and BOP power of a 1 MW system as a function of fuel utilization

Figure 35: Change in net power of a 1 MW system as a function of fuel utilization
A comparison of Figure 19 and Figure 36 shows that the hydrogen production is not really impacted as a result of changing the method of cooling. Predictably, the hydrogen decreases as a function of increased fuel utilization. Figure 37 presents the useful heat available.

![Hydrogen Flow Comparison](image)

Figure 36: Hydrogen flow of a 1 MW Tri-Generation system with integrated absorption chiller

The cooling produced by the single effect absorption chiller is presented in Figure 38 and shows the trend in cooling. The approach of mixing the chiller exhaust with the inlet to reach a specified inlet temperature of 250 °C was used in order to avoid injecting any unnecessary diluents into the HSU stream which will then need to be removed later by the PSA. The resultant cooling produced stays somewhat uniform as a function of fuel utilization. Figure 39 presents the coefficient of performance and, like the cooling, stays about the same for each fuel utilization.
Figure 37: Change in useful heat of a 1 MW system as a function of fuel utilization

Figure 38: Cooling produced by the integrated absorption chiller of a 1 MW system
Figure 39: Coefficient of performance of a 1 MW system as a function of fuel utilization

A comparison of Figure 22 and Figure 40 shows how the total system efficiency is affected as a result of integrating an absorption chiller with the HSU. The overall trend is flattened and there is no change in efficiency with varying fuel utilization, however, the highest efficiency achieved is somewhat lower. The efficiency of the baseline Tri-Generation case at 0.6 utilization yields total efficiency of 92.0% while the chiller supplemented case yields 85.9%. The reason an increase is not seen for the supplemented configuration is because a large amount of cathode inlet air is supplied by air pumped through the HSU for the baseline case. This air is preheated by the HSU and sent to the cathode with some additional air added as necessary. For the chiller supplemented configuration, that air is not available from the HSU since the absorption chiller uses water to cool significant portions of the HSU. As a result, more ambient air is needed in order to supply the cathode resulting in greater electrical parasitic losses to the system.
Table 7 and Table 8 present the product results for varying power levels for fuel utilization of 0.6 and 0.85 respectively. For the 0.6 utilization case, the efficiency stays relatively constant with an average of 84.9%, however the 0.85 utilization case has a much more variable efficiency. Figure 41 presents the efficiency comparison from the tables.
Table 7: Tri-Generation product results at 0.6 fuel utilization

<table>
<thead>
<tr>
<th>Nominal Power (MW)</th>
<th>Net Power (kW)</th>
<th>Hydrogen Flow (kg/hr)</th>
<th>Cooling (kW)</th>
<th>Heat (kW)</th>
<th>System Efficiency (%)</th>
<th>COP</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>822.0</td>
<td>11.2</td>
<td>114.9</td>
<td>142.4</td>
<td>85.9%</td>
<td>0.803</td>
</tr>
<tr>
<td>2</td>
<td>1646.3</td>
<td>22.4</td>
<td>231.4</td>
<td>283.8</td>
<td>85.8%</td>
<td>0.828</td>
</tr>
<tr>
<td>3</td>
<td>2466.6</td>
<td>33.8</td>
<td>345.3</td>
<td>425.8</td>
<td>85.9%</td>
<td>0.830</td>
</tr>
<tr>
<td>4</td>
<td>3378.0</td>
<td>38.6</td>
<td>469.0</td>
<td>566.5</td>
<td>83.8%</td>
<td>0.821</td>
</tr>
<tr>
<td>5</td>
<td>4187.3</td>
<td>49.9</td>
<td>596.6</td>
<td>708.2</td>
<td>84.1%</td>
<td>0.826</td>
</tr>
<tr>
<td>6</td>
<td>4941.2</td>
<td>64.7</td>
<td>722.5</td>
<td>850.5</td>
<td>84.9%</td>
<td>0.821</td>
</tr>
<tr>
<td>7</td>
<td>5757.6</td>
<td>75.4</td>
<td>840.7</td>
<td>992.2</td>
<td>84.8%</td>
<td>0.818</td>
</tr>
<tr>
<td>8</td>
<td>6575.5</td>
<td>86.0</td>
<td>950.9</td>
<td>1134.0</td>
<td>84.8%</td>
<td>0.814</td>
</tr>
<tr>
<td>9</td>
<td>7391.9</td>
<td>96.7</td>
<td>1057.5</td>
<td>1275.9</td>
<td>84.7%</td>
<td>0.809</td>
</tr>
<tr>
<td>10</td>
<td>8209.2</td>
<td>107.4</td>
<td>1157.9</td>
<td>1417.8</td>
<td>84.7%</td>
<td>0.805</td>
</tr>
</tbody>
</table>
Table 8: Tri-Generation product results at 0.85 fuel utilization

<table>
<thead>
<tr>
<th>Nominal Power (MW)</th>
<th>Net Power (kW)</th>
<th>Hydrogen Flow (kg/hr)</th>
<th>Cooling (kW)</th>
<th>Heat (kW)</th>
<th>System Efficiency (%)</th>
<th>COP</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>779.9</td>
<td>3.5</td>
<td>109.8</td>
<td>425.2</td>
<td>84.8%</td>
<td>0.807</td>
</tr>
<tr>
<td>2</td>
<td>1560.6</td>
<td>7.0</td>
<td>222.4</td>
<td>850.5</td>
<td>84.8%</td>
<td>0.824</td>
</tr>
<tr>
<td>3</td>
<td>2341.4</td>
<td>10.6</td>
<td>331.4</td>
<td>1275.8</td>
<td>84.9%</td>
<td>0.828</td>
</tr>
<tr>
<td>4</td>
<td>3118.9</td>
<td>14.1</td>
<td>442.6</td>
<td>1701.1</td>
<td>84.8%</td>
<td>0.830</td>
</tr>
<tr>
<td>5</td>
<td>3892.8</td>
<td>16.9</td>
<td>552.0</td>
<td>2126.4</td>
<td>84.4%</td>
<td>0.825</td>
</tr>
<tr>
<td>6</td>
<td>4668.2</td>
<td>20.3</td>
<td>657.9</td>
<td>2551.7</td>
<td>84.4%</td>
<td>0.823</td>
</tr>
<tr>
<td>7</td>
<td>5444.7</td>
<td>23.7</td>
<td>758.4</td>
<td>2977.1</td>
<td>84.3%</td>
<td>0.821</td>
</tr>
<tr>
<td>8</td>
<td>6220.4</td>
<td>27.0</td>
<td>855.4</td>
<td>3402.5</td>
<td>84.3%</td>
<td>0.817</td>
</tr>
<tr>
<td>9</td>
<td>6996.1</td>
<td>30.4</td>
<td>947.9</td>
<td>3828.0</td>
<td>84.3%</td>
<td>0.814</td>
</tr>
<tr>
<td>10</td>
<td>7771.8</td>
<td>33.8</td>
<td>1035.6</td>
<td>4253.5</td>
<td>84.3%</td>
<td>0.810</td>
</tr>
</tbody>
</table>

Figure 41: Efficiency of a chiller supplemented Tri-Generation system as a function of power
The comparison between the 0.6 utilization and 0.85 utilization case shows that there again is little change in overall efficiency as a function of power and fuel utilization. This result suggests that dynamic operation would be favorable for a load with varying demands between electricity, hydrogen, and heat. Figure 42 presents the change in COP as a function of nominal power.

![Figure 42: Coefficient of performance of an absorption chiller integrated into the hydrogen booster](image)

6. SUMMARY OF RESULTS

In summary, three different model configurations based on the SOFC bulk FORTRAN model were built and run. The SOFC bulk model was verified and then a baseline Tri-Generation system was implemented. The Quad-Generation model was then implemented followed by a Tri-Generation model with supplemented absorption chilling. The results from chapter 5 are summarized below.
6.1. Model Verification

A Tri-Generation model built in Aspen Plus was used as the baseline model to build three separate system configurations with various objectives. An SOFC was modeled as a bulk model in FORTRAN was used for the main energy conversion block of the model. This block was tested against the IEA benchmark for reformate inlet fuel at three different pressure levels. Agreement between the model and the IEA benchmark varied depending on pressure and current density. Overall, the relative error ranged from 0.01% and 8.4% (see Figure 11, Figure 12, and Figure 13 in 5.1 Model).

The same model was also compared with experimental results from Jiang and Virkar [37]. Their work tested different anode gas concentrations using different diluents. A comparison of the model output to Jiang and Virkar’s work showed that the model outputs a similar trend, but lower overall voltage for a given current density. An adjustment was made to the model output so that the lowest current density was equal for both plots and the trend remained the same. This comparison yielded relative errors between 1.7% and 5.1% (see Figure 14 and Figure 15).

6.2. Baseline Tri-Generation Model Results

The bulk SOFC model was used in the baseline Tri-Generation model which includes the SOFC balance of plant and hydrogen booster along with its associated blowers and cooling. The PSA was not explicitly modeled, but the assumed power requirements of the PSA are 30% of nominal fuel cell load [36]. Several cases were considered by varying fuel utilization and power capacity. Since the system model relied on a bulk SOFC model, results for different power capacities were generally similar. Therefore, results for the 1 MW system were presented (see 5.2 Baseline Tri-Generation Model Results).
The nominal power is the power output from the fuel cell block without consideration of balance of plant parasitic loads. Nominal power was compared against varying fuel utilization (between 0.6 and 0.85) which increases with increasing utilization. The balance of plant loads also increase, but at a different rate from the nominal power. This resulted in an overall net power reduction with increased utilization (see Figure 16 and Figure 17). Similarly, the available hydrogen decreased with increased utilization (see Figure 19). This result is due to less available hydrogen in the anode exhaust since more of it is used up in the generation of electricity. The increase in balance of plant requirements is a direct result of increased heat generated from the increased electrochemical reactions taking place with higher fuel utilizations. This translates to greater available useful heat (see Figure 20). Overall, the baseline Tri-Generation system efficiency decreases with increasing fuel utilization (see Figure 22).

A comparison of system efficiency as a function of power capacity was also presented. This result shows that for a given fuel utilization, the efficiency stays about the same across the different power capacities. Additionally, the 0.85 utilization is consistently lower than the 0.6 utilization (see Figure 23).

6.3. Quad-Generation Model Results

Several high temperature streams were analyzed to determine the best location for an absorption chiller. The three factors considered were temperature, mass flow, and whether the temperature could be altered without impacting the system operation. The combined system exhaust was a stream that had the best temperature, highest mass flow, and the change in temperature is a non-issue since there are no downstream components. Therefore, a double-effect absorption chiller was placed in the exhaust of the baseline Tri-Generation model to create a Quad-Generation model (see 5.3 Quad-Generation Model Results).
For higher power capacities, the absorption chiller model could not appropriately handle the higher mass flows of the exhaust. The results became unrealistic to a real system. For systems greater than 1 MW, the COP was varied as an additional parameter of the system operation.

The power results are similar to the baseline Tri-Generation model; the nominal power and balance of plant loads increase as fuel utilization increases. This resulted in the net power decreasing with increased utilization (see Figure 26 and Figure 27). Also, the hydrogen flow reduces as fuel utilization increases (see Figure 28 and Figure 29). At a fixed COP of 1.1, the system efficiency as a function of power capacity resembles that of the baseline Tri-Generation system except the system efficiency is reduced by about 5%. However, with a higher COP of 1.4, the system efficiency is slightly increased. There is also a significant increase in efficiency for the 0.85 utilization case. The results show that the efficiency difference between 0.6 and 0.85 utilization is much smaller than for the fixed 1.1 COP case (see Figure 30 and Figure 31).

Additionally, the comparison of heat and net power shows that there is a trade-off between the two. As net power decreases, useful heat increases, but slightly less so than the decrease of power. Cooling generated also increases with increased fuel utilization. This is due to the increased heat available to be converted to cooling via absorption chilling (see Figure 32 and Figure 33).

6.4. Supplemented Tri-Generation Model Results

The supplemented Tri-Generation model features an absorption chiller within the hydrogen booster. It essentially replaces an electric chiller which is used to cool the hydrogen enriched anode exhaust prior to the PSA inlet. The inlet requires low temperature and high pressure, but the stream leaves the low temperature water gas shift reactor at a high temperature and low pressure. An electric chiller is needed to provide the cooling after the stream has been
pressurized. This configuration replaces a double stage compression system with intercooling with a single stage compression. The heat gained from the compression is used in the absorption chiller to cool the PSA inlet stream as well as the stream entering the main compressor (see 5.4 Supplemented Tri-Generation Model Results).

The supplemented Tri-Generation model is similar to the other configurations in that the nominal power, balance of plant, and net power have similar results. The nominal power and balance of plant both increase with increased utilization. The net power decreases with larger utilizations (see Figure 34 and Figure 35). Also, the hydrogen flow decreases with fuel utilization (see Figure 36). The useful heat also increases as fuel utilization (see Figure 37). The cooling produced is not exported out of the system. Instead, it is used within the hydrogen booster only. For a 1 MW system, the amount of cooling varies between about 90 and 110 kW for a given utilization (see Figure 38). The cooling does not vary similarly to the other products because there is a similar mass flow going through the hydrogen booster for a given utilization. The difference is the concentration of various species which has a small impact on heat capacity of the stream. For lower utilizations, there is a higher percentage of hydrogen and a lower percentage of water. For higher utilizations, there is much less hydrogen and significantly more water. The coefficient of performance also doesn’t vary significantly with respect to fuel utilization (see Figure 39). However, there is some variance in COP as a function of nominal power (see Figure 42).

A comparison of the baseline Tri-Generation system to the chiller supplemented system yields overall lower system efficiency at low utilization. However, for varying fuel utilization, the supplemented system maintains relatively unchanged efficiency (see Figure 22 and Figure 40). This result suggests that dynamic operation of a Tri-Generation system with a built in
absorption chiller is possible. Specifically, for a time when heat is more important as a product, the utilization can be increased to generate more heat. The overall efficiency shouldn’t be affected, but the electrical efficiency will be affected. This result is similar to what was found for the Quad-Generation system. System efficiency, products, and chiller COP are also presented. The COP varies somewhat as a function of power (see Table 7, Table 8, Figure 41, and Figure 42).

7. CONCLUSIONS

Several conclusions can be made from the research presented above. Each major conclusion is followed by a brief descriptive paragraph:

1. The best location for integration of absorption chilling into a Quad-Generation system was identified as that of the overall system exhaust.

   An analysis on the various streams indicated that the system exhaust stream was the location for a chiller which provided the most cooling potential. The chiller was placed in the system exhaust and the model was run to verify that all inputs and outputs fell within expected ranges.

2. Power dependence on fuel utilization was mitigated by placing an absorption chiller in the hydrogen booster. The correlation of hydrogen generation to fuel utilization did not change.

   The HSU requires a high amount of cooling for the PSA inlet which was met by a simulated electric chiller in the baseline Tri-Generation system. A large amount of heat is available in the anode exhaust stream immediately following compression to 10 atm for the PSA inlet. This heat was used to drive a single effect absorption chiller.
to cool the PSA inlet stream with chilled water. This configuration removed the
electric chiller load, potentially increasing system efficiency. The model was run at
varying nominal power capacities and varying fuel utilization. The results showed
that the electrical efficiency actually decreased since less preheated air was available
for the cathode inlet; however, the system efficiency was not affected by varying fuel
utilization. This result suggests that the proposed configuration would allow for more
flexible power following schemes without a varying impact on efficiency.

3. Cooling, heating, hydrogen, and power were maximized by placing an absorption
chiller in the system exhaust.

As mentioned above, cooling is maximized by being placed within the overall system
exhaust. This location had no impact on any downstream components and therefore
provided an extra useable product at no extra fuel cost. Electrical efficiency was not
impacted, nor was hydrogen efficiency. The overall system efficiency was increased
significantly and there was no impact on the efficiency as the fuel utilization was
varied.

Each of the objectives of this work was met and the results suggest some interesting findings
that can motivate future work on the subject. Namely, integration of an absorption chiller within
a Tri-Generation hydrogen booster reduces the negative impact that increased fuel utilization has
on system efficiency. The same result is true for the Quad-Generation case where an absorption
chiller is added to the exhaust stream for a fourth product which can be exported along with
electricity, hydrogen, and heat. An additional benefit of the Quad-Generation case is that the
overall system efficiency is increased significantly with the added product and without adverse
impact on system operation. These results suggest that inclusion of an absorption chiller could
enable dynamic operation of a system where varying loads of cooling, heating, hydrogen, and power are required without impact to system efficiency. A method to match these varying loads would be to simply adjust the target fuel utilization of the fuel cell. For example, a lower utilization would favor electricity and hydrogen production. A higher utilization would favor heating and cooling at the cost of electrical and hydrogen generation efficiency. The results also suggested that efficiency doesn’t change significantly with varying levels of power. Though, a spatially resolved model would be better equipped to address that suggestion more thoroughly.

8. RECOMMENDATIONS

As mentioned above, dynamic operation without impacting the system efficiency is suggested from the results of this work. These results motivate the need for further work on these system concepts to fully characterize their potential impact. The model used in this work is not suited to simulate a dynamic system in which varying levels of cooling, heating, hydrogen, and power are required. MATLAB Simulink is one tool, among others, that could be used to model a Tri-Generation system or Quad-Generation system under dynamic loading. The dynamic response, coupled with a spatially and temporally resolved model would be able to accurately characterize a real system in order to verify or refute the results of this work. If the results are verified in this manner, then this strongly suggests a direction in which a polygenerating system could be realized. Furthermore, a spatially and temporally resolved model could verify the results regarding power capacity. This knowledge could give a better indication of how big a real system could effectively be made.

An important consideration for the validity of these system configurations are the economics of building and operating them. Future research needs to be done in order to quantify the total
capital costs along with operating and maintenance costs of such a system. The results of such an analysis are essential in order to characterize viability of realizing these systems. Improved efficiency reduces operation costs by using less fuel for more products, but may do little to increase reliability or bring down capital costs. Ultimately, a comparison of the above systems with comparable state-of-the-art systems, such as gas turbines and electric chillers, would need to be completed in order to create a clear picture of the economic viability of this system.

Another consideration that is becoming increasingly important is the environmental impact of the system. Not only are emissions over the lifetime of the system important, but also the energy and materials required for its entire life cycle. A life cycle analysis on the environmental impact of the system will help determine whether the system is capable of providing an improvement to the environment in a significant fashion compared to comparable state-of-the-art systems, such as gas turbines and electric chillers.

If the above analyses prove worthwhile, a small demonstration project should be constructed to achieve its own set of goals and objectives. This project, relying on this work and the future work mentioned above, will pave the way to future commercial scale systems.
9. REFERENCES


