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**PROCESS DESIGN, DYNAMICS, AND TECHNO-ECONOMIC ANALYSIS OF A  
SUSTAINABLE COAL, WIND, AND SMALL MODULAR NUCLEAR REACTOR  
HYBRID ENERGY SYSTEM**

**by**

**KYLE LEE BUCHHEIT**

**A DISSERTATION**

**Presented to the Graduate Faculty of the**

**MISSOURI UNIVERSITY OF SCIENCE AND TECHNOLOGY**

**In Partial Fulfillment of the Requirements for the Degree**

**DOCTOR OF PHILOSOPHY**

**in**

**CHEMICAL ENGINEERING**

**2015**

**Approved by:**

**Dr. Joseph Smith, Advisor**

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**Dr. John Singler**

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## **PUBLICATION DISSERTATION OPTION**

This dissertation consists of the following three articles that have been submitted for publication as follows:

Techno-Economic Analysis of a Sustainable Coal, Wind and Nuclear Hybrid Energy System, Pages 2-22 have been submitted to ENERGY.

Dynamic Process Modeling of a Sustainable Coal, Wind, and Small Modular Reactor Hybrid Energy System, Pages 23-40 have been submitted to RENEWABLE ENERGY.

Production Possibilities of a Sustainable Coal, Wind, and Small Modular Reactor Hybrid Energy System, Pages 41-99 are intended for submission in ENERGY ECONOMICS.

This dissertation follows formatting rules as set forth by the Missouri University of Science and Technology.

## ABSTRACT

The availability of cheap electricity is one of the biggest factors for improving quality of life. With the debate on the effects of carbon dioxide emissions continuing, several countries have either implemented or are considering the reduction of emissions through various economic means. The inclusion of a monetary penalty on carbon emissions would increase the prices of electricity produced by carbon-based sources. The push for large-scale renewable sources of energy has met problems with regards to energy storage and availability. The proposed coal, wind, and nuclear hybrid energy system would combine a renewable energy source, wind, with traditional and stable energy sources, coal and nuclear, to create an integrated and sustainable system. A next generation small modular nuclear reactor will be evaluated. The coal system will use a pressurized circulating fluidized bed system, which can utilize both coal and biomass as a carbon feedstock. This system also employs a high temperature steam co-electrolysis unit for the utilization of carbon dioxide emissions for the production of synthetic gas which can be used in the production of transportation fuels or chemicals.

The coal and nuclear systems were first analyzed at steady state by utilizing the Aspen Plus simulation software. The two systems were integrated with an existing high temperature steam electrolysis model. This system was reconciled and simplified. The simplifications to the model allowed for export from Aspen Plus into Aspen Dynamics. Once in the Dynamics simulation software, wind and grid demand models were developed to simulate a full year of power generation, power consumption, and chemical production. The simulation results were used to generate production possibilities and to compare the hybrid system to conventional coal technologies by levelized costs.

## ACKNOWLEDGEMENTS

I owe my deepest gratitude to my advisor Dr. Joseph D. Smith. He accepted me into his research group when he first arrived at Missouri S&T. Without him, I would not have been able to continue my pursuit of a Ph.D. degree. With him I have grown both academically and personally, learning about what it takes to not only be professional, but how to treat others with respect and care about others like family. With the trust he placed in me to complete my work, I know I owe him a great deal for allowing me to travel to China and meet the woman who became my wife.

I would like to show my thanks to all the remaining members of my committee. Dr. Al-Dahhan supported me as one of four undergraduates entering graduate school for the Chancellor's Fellowship which has taken care of my tuition. Dr. Book not only introduced me to mathematical modeling (Mathcad) but also helped me with a teaching opportunity during a difficult transition period. Dr. Gelles worked with me as an undergraduate to combine my love of engineering and economics into a double major and continued to help me throughout my graduate work. Lastly, Dr. Singler expanded my knowledge of mathematical modeling with programming, techniques that shaped my entire graduate work and now the type of work that I am interested in.

I would like to thank the friends I have made while working at the ERDC: Uday, Chen, Hassan, Anand, Prashant, Jeremy, Vivek, Shyam, Haider, Teja, Jia, Han, and many others. We've traveled together, worked together, struggled together, and in the end we all learned from one another. Finally, I have to thank my wife, Jing Zhang, for encouraging me to "stop being so lazy and get some work done!"

## TABLE OF CONTENTS

	Page
PUBLICATION DISSERTATION OPTION .....	iii
ABSTRACT .....	iv
ACKNOWLEDGEMENTS .....	v
LIST OF ILLUSTRATIONS .....	viii
LIST OF TABLES .....	x
 SECTION	
1. INTRODUCTION .....	1
 PAPER	
I. TECHNO-ECONOMIC ANALYSIS OF A SUSTAINABLE COAL, WIND AND NUCLEAR HYBRID ENERGY SYSTEM .....	2
ABSTRACT .....	2
1. INTRODUCTION AND BACKGROUND .....	3
2. METHODOLOGY .....	5
3. SIMULATION CONVERGENCE .....	8
4. INITIAL RESULTS .....	11
5. FINAL RESULTS .....	16
6. FUTURE WORK .....	22
II. DYNAMIC PROCESS MODELING OF A SUSTAINABLE COAL, WIND, AND SMALL MODULAR REACTOR HYBRID ENERGY SYSTEM .....	23
ABSTRACT .....	23
1. INTRODUCTION AND BACKGROUND .....	24

2. METHODOLOGY.....	26
3. RESULTS .....	35
4. FUTURE WORK.....	40
III. PRODUCTION POSSIBILITIES OF A SUSTAINABLE COAL, WIND, AND SMALL MODULAR REACTOR HYBRID ENERGY SYSTEM .....	41
ABSTRACT .....	41
1. INTRODUCTION AND BACKGROUND.....	43
2. METHODOLOGY.....	45
3. SIMULATION RESULTS .....	51
4. ECONOMIC EVALUATION .....	60
5. CONCLUSIONS.....	66
6. FUTURE WORK.....	67
APPENDICES	
A. HYBRID ENERGY SYSTEM DYNAMIC SIMULATION RESULTS .....	68
B. HYBRID ENERGY SYSTEM ECONOMIC EVALUATIONS .....	81
SECTION	
2. CONCLUSIONS.....	100
APPENDICES	
A. RIGOROUS STEADY STATE ASPEN PLUS INPUT .....	101
B. CONSOLIDATED STEADY STATE ASPEN PLUS INPUT .....	130
REFERENCES .....	149
VITA .....	151



## LIST OF ILLUSTRATIONS

Figure	Page
 PAPER I	
1.1. World energy consumption by resource type [1].....	4
2.1. Diagram of a Pressurized Circulating Fluidized Bed combustion system [4]. .....	5
4.1. Initial Overall Hybrid Energy System Process Flow Diagram. ....	12
4.2. Initial Pressurized Circulating Fluidized Bed combustor flow diagram. ....	12
4.3. Initial Benfield process flow diagram. ....	14
4.4. High Temperature Steam Electrolysis, outer hierarchy (left), inner hierarchy (right). ....	14
5.1. Revised Pressurized Circulating Fluidized Bed. ....	17
5.2. Small Modular Reactor Flow Diagram. ....	18
5.3. Benfield Process Flow Diagram. ....	18
 PAPER II	
1.1. Monthly Wind Energy Production [13]. ....	25
2.1. Steady State Model. ....	27
2.2. PCFB Hierarchy.....	27
2.3. Carbon Dioxide Capture. ....	28
2.4. Nuclear Small Modular Reactor. ....	29
2.5. High Temperature Steam Electrolysis, Outer Hierarchy. ....	30
2.6. High Temperature Steam Electrolysis, Inner Hierarchy. ....	30
2.7. Reconciled PCFB.....	31
2.8. Simplified High Temperature Steam Electrolysis. ....	32
2.9. Dynamic Overall Hybrid Energy System. ....	34

2.10.	Dynamic High Temperature Steam Electrolysis Hierarchy.....	34
3.1.	Operating Curve for HTSE Reactants.....	37
3.2.	Grid Demand.....	38
3.3.	Dynamic Wind Power Generated. ....	38
3.4.	Dynamic Syngas Production.....	39

### PAPER III

2.1.	Average Wind Speeds from National Wind Technology Center.....	46
2.2.	Scaled Grid Demand from Southwest Power Pool. ....	47
2.3.	Wind Turbine Model Power Generated. ....	48
2.4.	Real Data Modified Process Flow Diagram of Aspen Dynamics Model. ....	49
3.1.	Power Generated vs. Grid Demand for Base System. ....	51
3.2.	Peak Power Demand for Base Hybrid System.....	52
3.3.	Carbon Dioxide Emissions for Base Hybrid System. ....	54
3.4.	Syngas Production of Base Hybrid System. ....	54
3.5.	Grid Demand versus generation comparison. ....	55
3.6.	Peaking power comparison. ....	56
3.7.	Carbon dioxide emissions comparison. ....	57
3.8.	Syngas produced comparison.....	58

## LIST OF TABLES

Table	Page
 PAPER I	
1.1. World Carbon Dioxide emissions [2]. .....	4
2.1. Sargas technology [9].....	7
4.1. Selected Initial Stream Results. ....	15
5.1. Selected Stream Results. ....	20
5.2. Stand-alone Efficiencies. ....	20
5.3. Levelized Costs of Electricity [10]. ....	21
 PAPER II	
3.1. High Temperature Steam Electrolysis Conversion. ....	36
3.2. High Temperature Steam Electrolysis Reactants. ....	37
 PAPER III	
2.1. Hybrid Systems Evaluated. ....	50
3.1. Yearly Gases Emitted and Produced.....	59
4.1. Levelized Cost of Electricity.....	61
4.2. Base Hybrid System Levelized Cost Comparisons (A). ....	63
4.3. Base Hybrid System Levelized Cost Comparisons (B). ....	64
4.4. Value of Syngas for Base Hybrid System.....	65
4.5. Syngas Sale Price for Base Hybrid System. ....	65

## **1. INTRODUCTION**

This work is divided into four phases: Phase 1 – Initial Design and Analysis, Phase 2 – Detailed Process Design, Phase 3 – Dynamic Process Design, and Phase 4 – Real Data and Full Analysis. Phase 1 investigates the overall initial design considerations of the hybrid energy system. It contains the initial model for the pressurized circulating fluidized bed (PCFB), carbon dioxide absorption options, the full high temperature steam electrolysis model, and baseline results. Phase 2 contains updates to the PCFB model, the nuclear small modular reactor (SMR) model, a finalized Benfield Process model for carbon dioxide absorption, and updated model results. Phase 3 has small modifications to the electricity generating turbines in the PCFB, SMR water cycles, overall system consolidations, initial electricity use logic, and sample dynamic results that include wind. Phase 4 integrates real world grid demand and dynamic wind data, runs the hybrid system for a full year, contains the production possibilities of the system, and concludes with system cost comparisons to conventional technologies.

Both Phase 1 and Phase 2 depict the construction of the Aspen Plus steady state model and are presented in the article titled “Techno-Economic Analysis of a Sustainable Coal, Wind and Nuclear Hybrid Energy System.” Phase 3 relates the transition from the Aspen Plus steady state model into the Aspen Dynamics dynamic model and is presented in the article titled “Dynamic Process Modeling of a Sustainable Coal, Wind, and Small Modular Reactor Hybrid Energy System.” Phase 4 uses the dynamic model with real world data to generate production possibilities and to perform an economic analysis which is presented in the article titled “Production Possibilities of a Sustainable Coal, Wind, and Small Modular Reactor Hybrid Energy System.”

## **PAPER**

### **I. TECHNO-ECONOMIC ANALYSIS OF A SUSTAINABLE COAL, WIND AND NUCLEAR HYBRID ENERGY SYSTEM**

#### **ABSTRACT**

The availability of cheap electricity is one of the biggest factors for improving quality of life. The push for large-scale renewable sources of energy has met problems with regards to energy storage and availability. The proposed coal, wind and nuclear hybrid energy system would combine a renewable energy source, wind, with traditional and stable energy sources, coal and nuclear, to create an integrated, resilient, and sustainable system. A next generation small modular nuclear reactor is considered together with a pressurized circulating fluidized bed coal combustion system, which also utilizes biomass as a feedstock. This system employs a co-electrolysis unit for utilization of carbon dioxide as a feedstock for the production of synthetic gas and subsequently fuels and chemicals. A techno-economic analysis of the proposed system has been performed, along with a thermodynamic analysis of overall efficiency and sustainability.

## 1. INTRODUCTION AND BACKGROUND

Modern societies require the use of energy to perform large tasks efficiently. Since the industrial revolution and the introduction of the combustion engine, fossil fuels have been the main source of energy. Since then, countries with inexpensive sources of fossil energy have taken a major economic role in the world. Due to differences in culture, economic standing, government ideologies, etc., conflicts have arisen over the control of these fossil fuel resources. Energy policy itself in each country is therefore closely tied to economic and defense policy.

Total energy consumption sorted by source (Figure 1.1) throughout recent history shows that fossil energy (i.e., oil, natural gas, and coal) makes up the vast majority of the world's energy production. Although non-carbon based energy sources are available, their contribution is increasing slowly, leaving us heavily dependent on carbon for our energy needs. Due to recent changes in public opinion over nuclear power, most likely due to recent events at the Fukushima nuclear plant in Japan, there has been a 6.9% drop in nuclear power use from 2011 to 2012 [1], though it remains the only large scale “carbon-free” energy resource.

The approximate amount of global carbon dioxide emissions has more than doubled over the past forty years (Table 1.1). This increase in emissions can be directly related to the increase in energy consumption. On March 15th, 2012, U.S. President Barack Obama spoke out about the future of energy in the United States, when he recommended utilizing an “all-of-the-above” approach to securing energy stability [3]. This approach involves using some or all of the available energy sources on hand to match consumption demand. This strategy has led to the development of the Hybrid

Energy System concept which combines available traditionally used carbon based sources with renewable resources.

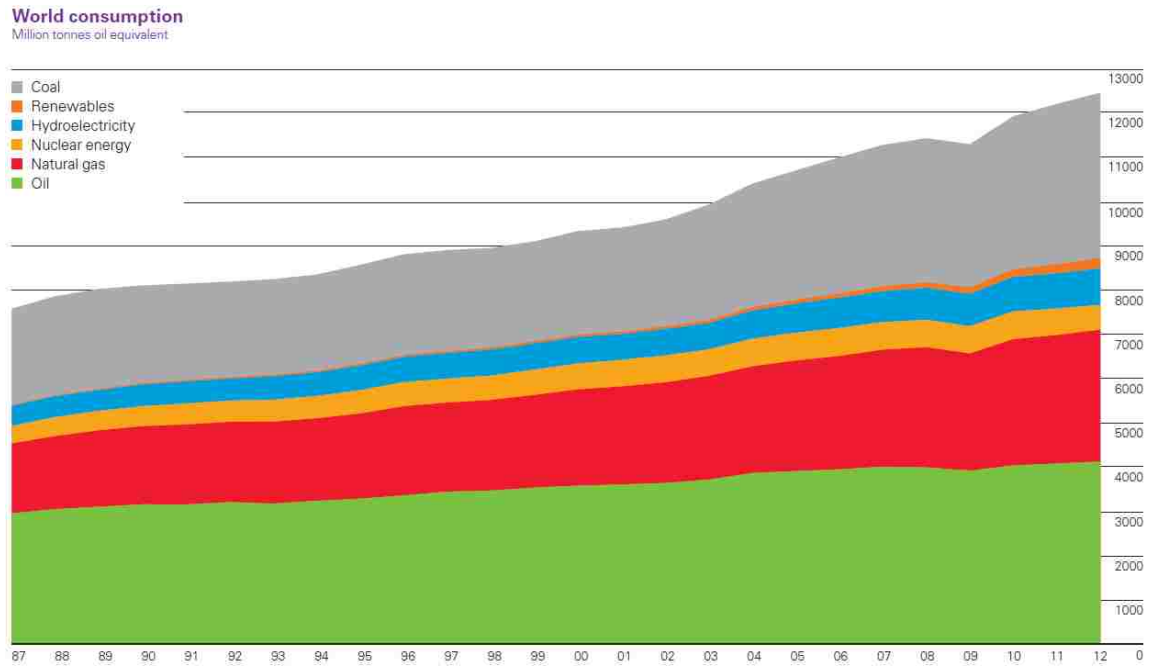


Figure 1.1. World energy consumption by resource type [1].

Table 1.1. World Carbon Dioxide emissions [2].

### CO<sub>2</sub> emissions: Sectoral Approach

million tonnes of CO <sub>2</sub>											
	1971	1975	1980	1985	1990	1995	2000	2005	2008	2009	% change 90-10
World *	14 064.8	15 668.5	18 042.2	18 623.5	20 973.9	21 843.8	23 509.1	27 187.4	29 483.0	28 946.7	44.4%

\* Total world includes non-OECD total, OECD total as well as international marine bunkers and international aviation bunkers.

## 2. METHODOLOGY

To use existing carbon based energy resources, a coal/biomass-fed pressurized circulating fluidized bed (PCFB) combustor was evaluated. The PCFB is capable of using lower quality (high sulfur, high ash) coal with minimal loss in efficiency and is capable of high thermal efficiencies (~50%). This system also enjoys smaller sizes of equipment due to increased operating pressures while generating pressurized flue gases [4] (see Figure 2.1).

The Westinghouse small modular reactor (SMR) design was selected to represent the next generation of nuclear reactors. Each reactor converts 800 MWt to approximately 225 MWe. The Westinghouse design, like other SMR designs, has improved safety features, utilizing natural convective and gravitational forces to remove reactor heat for up to 7 days without an external backup power source [5, 6].

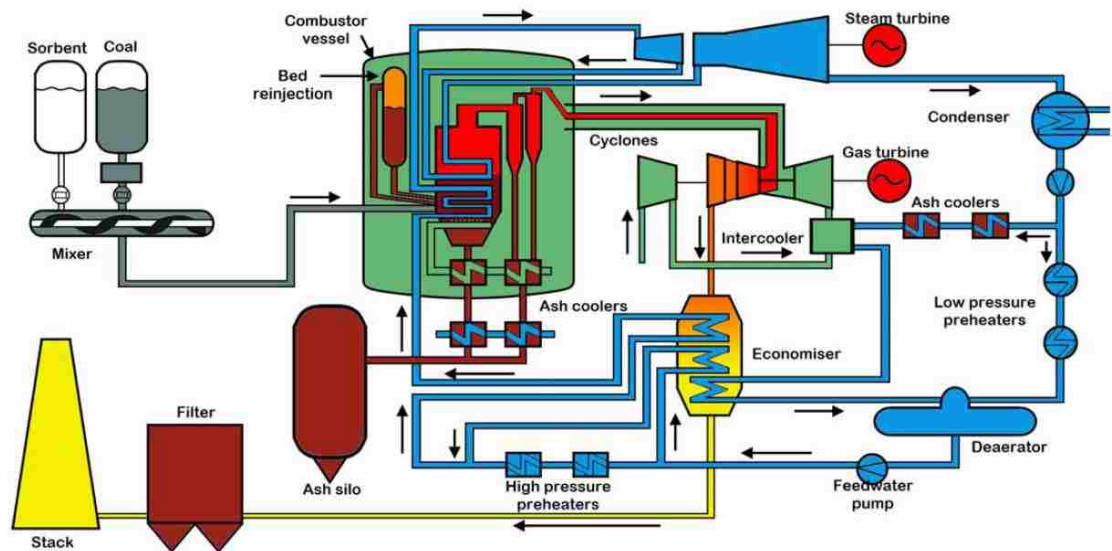


Figure 2.1. Diagram of a Pressurized Circulating Fluidized Bed combustion system [4].



The pressurized flue gas exiting the PCFB is fed to various air scrubbing units to remove particles, sulfur and nitrogen compounds, and carbon dioxide using a Benfield process. This carbon dioxide removal process uses a recycled aqueous potassium carbonate stream supported with piperazine for absorbing carbon dioxide from the flue gas. Cleaned flue gas is exhausted to the atmosphere while the carbon dioxide solution is processed in a double matrix stripper to create a pure stream of carbon dioxide that is sent to a high temperature steam co-electrolysis unit. This configuration removes and utilizes more than 90% of the carbon dioxide from the flue gas [7].

The pure carbon dioxide stream is sent for processing along with steam into the high temperature steam electrolysis (HTSE) unit. The unit splits the steam into oxygen and hydrogen, and then is modeled by a water-gas-shift reaction to produce carbon monoxide [8]. The combined hydrogen and carbon monoxide form synthesis gas that can be sent on for further processing. The oxygen produced is carried out by a sweep-gas that feeds back to the PCFB process, further enhancing combustion efficiency in the system.

The renewable portion of the hybrid energy system could be filled by any resource based on performance, technology, economics, etc. This system employs wind due to the maturity of the technology. One of the issues associated with wind energy is its highly dynamic nature. Since wind patterns are unpredictable, the energy provided by wind is often difficult to utilize. With such a time dependent nature, it is impossible to properly model wind energy using a steady state process simulation tool. Every process outlined above is modeled in Aspen Plus to assess the overall system efficiency. The PCFB combustor was modeled after the performance of the Alstom P200 operating in

Europe (Table 2.1) [9]. The plant performance was included in the Aspen Plus model to complete the material and energy balance focusing on carbon dioxide with a total of 200 MWe energy production. Utilizing design specifications and in-line FORTRAN programming were key to ensuring the material and energy balances closed along with overall simulation convergence.

Table 2.1. Sargas technology [9].

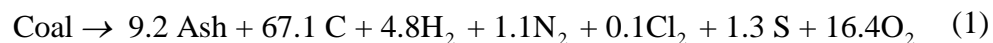
<i>Feature (100 MW unit block)</i>	<i>Value</i>	<i>Comments:</i>
Overall plant efficiency (HHV) - %	39.30	Not accounting for CO <sub>2</sub> compression
Fuel supply kg/s	7.5	Dry coal. HHV equals 33.927 MJ/kg
Unit power - MW <sub>e</sub>	100	Full plant 400 MW <sub>e</sub> requiring 4 unit blocks
CO <sub>2</sub> generated – kg/s	26.47	
CO <sub>2</sub> captured – kg/s	23.92	Thus emitting 2.5518 kg/s CO <sub>2</sub>
CO <sub>2</sub> capture rate - %	90.36	

### 3. SIMULATION CONVERGENCE

The proposed hybrid energy system has multiple, integrated iterative loops that pose a significant challenge to simulation convergence. The small modular reactor required an internal water recycle for steam generation. The carbon dioxide capture unit uses an internal recycle of the solvent. The co-electrolysis unit has a recycle stream of hydrogen and carbon monoxide for the equilibrium reactions. Finally, the overall system has a recycle stream of oxygen enriched air from the co-electrolysis unit to the coal combustor.

The overall hybrid model energy system was developed in modules to first gain pseudo steady-state solutions for use as initial conditions. Each individual module is run separately before being combined utilizing the custom user model hierarchy blocks in Aspen Plus. The SMR and PCFB were run first before being fed into the carbon dioxide capture unit, then finally the conditions were fed into the co-electrolysis unit. To reduce simulation time and improve convergence, the inner loop of the SMR steam cycle was simply modeled by matching the conditions of the inlet and outlet streams, rather than running the loop iteratively.

The initial focus of this analysis considered the flow of carbon through the units. Carbon fed as coal is extracted and combusted into carbon dioxide then captured and utilized. The ultimate coal analysis can be used to first break the pseudo component of coal into chemical species represented by the following equation on a mass basis:

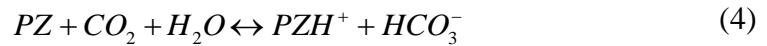


Using this basis, chemical reactions take place, most notably, the conversion into carbon dioxide:



Since the recycle loop of the solvent for the carbon dioxide capture unit is sensitive to composition change, a stream matching scheme is insufficient. Instead, a design spec is set in conjunction with a Multiply block inside of Aspen Plus. As the simulation runs, the design spec modifies the factor inside the Multiply block. This block manipulates the stream of fresh solvent, starting with all fresh solvent and eventually solving the iterative loop allowing for the recycled solvent. After convergence, the modified flow of fresh solvent entering the loop is determined.

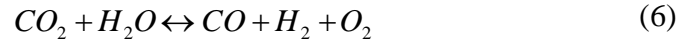
The absorber and stripper unit utilizing aqueous potassium carbonate supported by piperazine (PZ) is modeled by using the following three equilibrium reactions:



Using these reactions with a 90% minimum capture rate of carbon dioxide, the design spec is set to allow 1 kg H<sub>2</sub>O for every 1.4889 moles of CO<sub>2</sub>.

The co-electrolysis model has been fine tuned to accept approximately a third of the carbon dioxide produced by the PCFB and is then converged at a specific steady state. To preserve convergence, another design spec is set to modify a flow splitter block to allow only a certain, preset amount of carbon dioxide into the unit. The recycle stream of carbon monoxide and hydrogen gas is also set with a purge stream to maintain steady

flow rates. The series of RGibbs and RStoic reactors operating inside of the co-electrolysis block follow the overall reaction:



As with the carbon dioxide capture unit, a design spec and Multiply block combination is configured to modify the inlet of air to the PCFB combustor. This design spec changes the factor inside the Multiply block to maintain the stoichiometric amount of oxygen required for combustion inside the PCFB hierarchy. The addition of these design specs and the modularity of the units allows the overall hybrid energy system model to converge in a timely manner utilizing initial conditions. The Secant Method is the non-linear solver utilized in this simulation.

$$x_{k+1} = x_k - \frac{f(x_k)(x_k - x_{k-1})}{f(x_k) - f(x_{k-1})} \quad (7)$$

The previous equation illustrates one of the strengths of this method and why it was chosen. Here  $x_k$  represents the current solution,  $x_{k-1}$  the previous solution,  $x_{k+1}$  the next solution and  $f(x_i)$  the function evaluated at point  $x_i$ . To obtain the next solution, information about the function at the current and previous steps is required to solve the iterative step. The key feature is that the method does not require information about the derivative of the function, nor does it implicitly depend on the next solution.

#### 4. INITIAL RESULTS

Each operational unit (PCFB, Benfield process, HTSE, SMR) was individually completed and converged prior to total process hybridization (Figure 4.1). Each system was inserted into its own Aspen Plus Hierarchy block for different simulation options and overall simplicity. In the process, coal and air are fed into the PCFB combustor, producing electricity and an effluent stream. The stream is then sent into the Benfield air scrubber to generate a pure CO<sub>2</sub> stream. The CO<sub>2</sub> stream is then prepared for the HTSE unit by modifying its temperature and pressure. The product synthesis gas is then ready for further application and the produced oxygen is then recycled back for air enrichment into the PCFB combustor. For convergence efficiency, the recycle stream was specified as a major tear stream variable, and an Aspen Plus multiplier block was used to change the inlet flow rate of air until a final solution of inlet oxygen for combustion was found.

For the modeling of the PCFB unit, inlet coal was taken through a yield reactor to generate the atomic species present in the coal. A splitter was used to remove the ash and moisture from the coal elements, passing the reacting species to a stoichiometric reactor, generating heat and carbon dioxide from the equilibrium combustion reactions of coal and enriched air. The heat stream was processed through another heat splitter to generate the proper amount of electricity. Since each P200 combustor is rated at 100 MWe, two models were used in parallel and combined. (See Figure 4.2 for a layout of the described PCFB model)

A stream containing 4 molal K<sup>+</sup> ions / 4 molal piperazine aqueous solution is used to separate the carbon dioxide from the PCFB unit in the Benfield process unit. An Aspen Plus multiplier block was used to adjust the aqueous stream to allow for 1 kg

water per 1.489 moles of carbon dioxide to achieve 90% carbon dioxide removal. The absorbed solution was then split fed into two stripping columns to recover the absorbent and generate the pure carbon dioxide stream (See Figure 4.3).

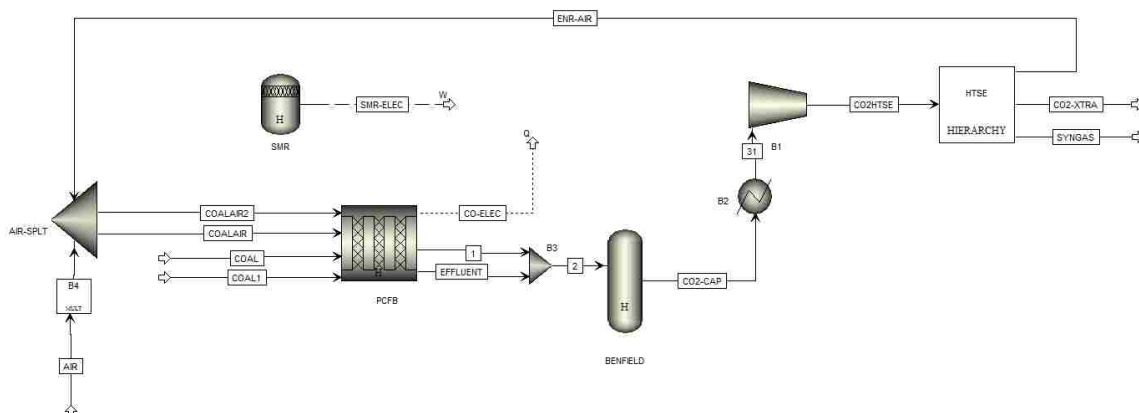


Figure 4.1. Initial Overall Hybrid Energy System Process Flow Diagram.

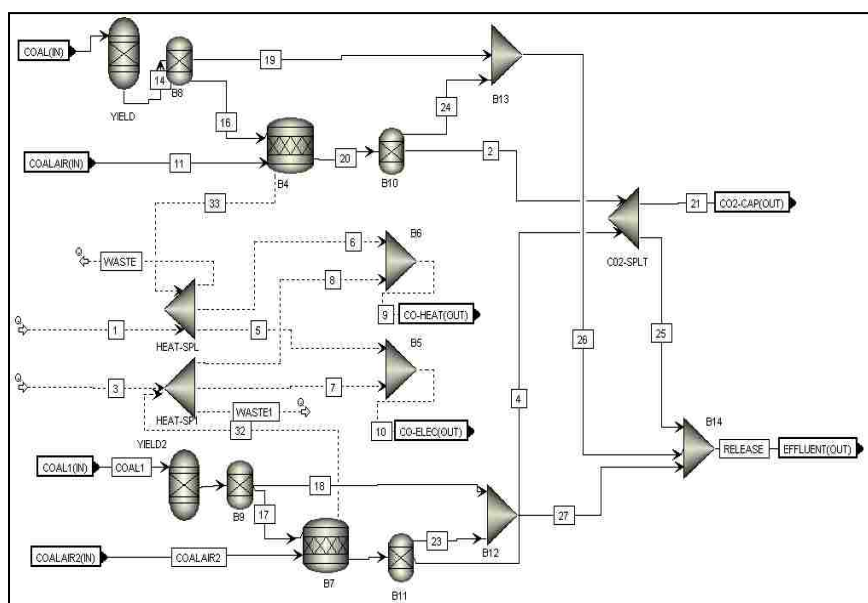


Figure 4.2. Initial Pressurized Circulating Fluidized Bed combustor flow diagram.

The pure CO<sub>2</sub> stream was fed into the HTSE unit along with water and air used as a sweep gas. The CO<sub>2</sub>, water, and air are modified to reach desired temperatures and pressures in the outer HTSE hierarchy, before being fed to the modeled reactors in the inner hierarchy (see Figure 4.4). The model used an Aspen Plus RGibbs reactor, RStoic reactor, and Sep blocks to mimic the reactions occurring inside an actual HTSE. The RGibbs reactors follow thermodynamic principles to reach equilibrium based on chemical species present while the RStoic reactor follows the water-gas-shift reaction. In-line FORTRAN code generates the amount of thermal energy and electrical energy necessary to operate the unit.

Table 4.1 displays several selected key streams throughout the process. Important to note is that the overall process produces approximately 4,332 kmol/hr of carbon dioxide, of which nearly one third is converted into syngas via the current model. The enriched air stream that was the sweep gas that had collected the oxygen produced in the HTSE is nearly half oxygen and half nitrogen. The enriched air stream being mixed with air for the PCFB combustion process creates a coal air feed that is nearly 25% oxygen, versus 21% for atmospheric air.



Figure 4.4. High Temperature Steam Electrolysis, outer hierarchy (left), inner hierarchy (right).

Table 4.1. Selected Initial Stream Results.

Stream Name	PCFB Flue Gas	CO <sub>2</sub> to HTSE	Enriched Air	Unused CO <sub>2</sub>	Syngas	Coal Air
Total Flow (kmol/hr)	16,053	3,899	4,986	2,544	4,058	38,457
Component Flows (kmol/hr)						
CO <sub>2</sub>	4,332	3,899	-	2,544	183	-
CO	-	-	-	-	1,173	-
N <sub>2</sub>	9,444	-	2,493	-	-	28,936
H <sub>2</sub>	1,847	-	-	-	2,487	-
O <sub>2</sub>	397	-	2,493	-	-	9,522
H <sub>2</sub> O	-	-	-	-	215	-
Mole Fractions						
CO <sub>2</sub>	0.2699	1.0000	-	1.0000	0.0450	-
CO	-	-	-	-	0.2891	-
N <sub>2</sub>	0.5883	-	0.5001	-	-	0.7524
H <sub>2</sub>	0.1150	-	-	-	0.6129	-
O <sub>2</sub>	0.0248	-	0.4999	-	-	0.2476
H <sub>2</sub> O	-	-	-	-	0.0530	-

## 5. FINAL RESULTS

The initial results provide a baseline for modifying the Hybrid Energy System model to increase its robustness in terms of computational efficiency and accuracy. The modified model included a simplified SMR model, streamlined PCFB model with more realistic thermodynamics, and changes made to recycle streams. The updated results reflect the hybridization of the enriched air stream changing the chemical equilibrium from the initial stoichiometric based results.

The preliminary model using stoichiometric data to match Sargas Technology results only works if the hybrid model uses atmospheric air. Since the enriched air recycle introduces higher levels of oxygen than is normally present in atmospheric air, a different approach was taken to better capture the combustion products (Figure 5.1). The updated model was built using two parallel units to provide the total 200 MWe. The inlet coal first enters a yield reactor to generate the atomic species present based on the ultimate coal analysis. The coal species and compressed enriched air are fed into an RGibbs reactor that determines combustion products based on thermodynamic equilibrium, thereby taking into account the enriched oxygen as opposed to using a stoichiometric based approach to the reactions. The reaction products were sent through a cyclone to return any non-combusted material back to the reactor before being sent as effluent to the carbon dioxide capture unit. In addition to the changes made to the reactor, a steam turbine was added to more accurately transform the thermal energy derived from combustion into electrical energy.

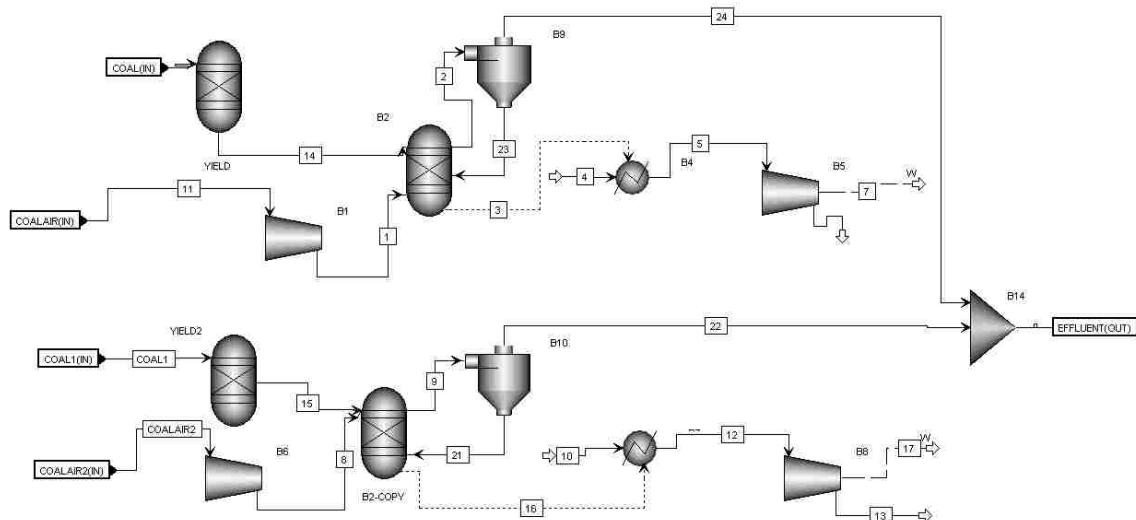


Figure 5.1. Revised Pressurized Circulating Fluidized Bed.

The SMR was initially modeled by simply converting a heat stream into a work (electrical energy) stream with a waste heat stream. This method did not capture the amount of water necessary to perform this function nor allow for steam to be utilized elsewhere in the system. The updated model, shown in Figure 5.2, uses two water cycles that mimic the cycles in the SMR. The inner loop takes the thermal energy generated by the nuclear core and transfers this energy to the outer loop to generate steam which in turn generates electricity in a turbine. Instead of using a closed loop recycle system, the streams are reconciled to ensure matching state variables to reduce computational requirements.

The recycle stream in the Benfield process (Figure 5.3) was handled similarly to the water loops in the SMR. By reconciling the streams as opposed to having a full recycle, the system takes much less computation time while retaining similar results as originally obtained.

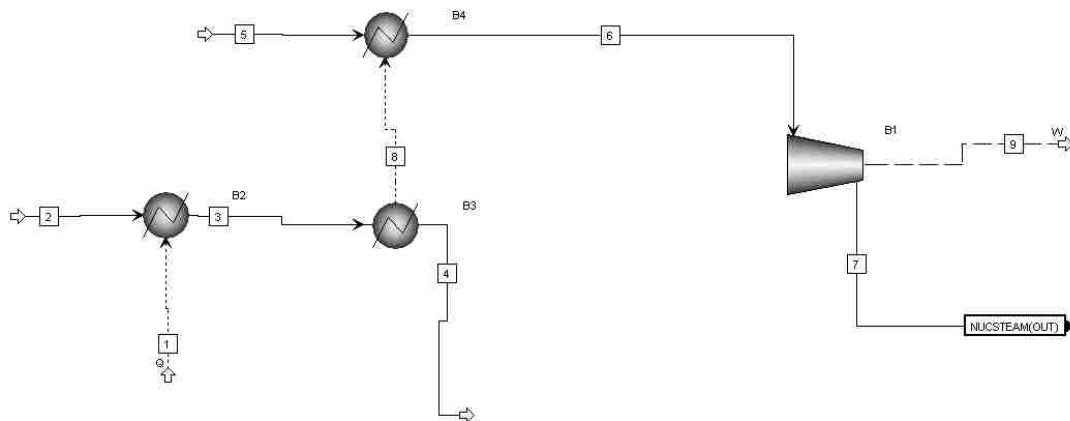


Figure 5.2. Small Modular Reactor Flow Diagram.

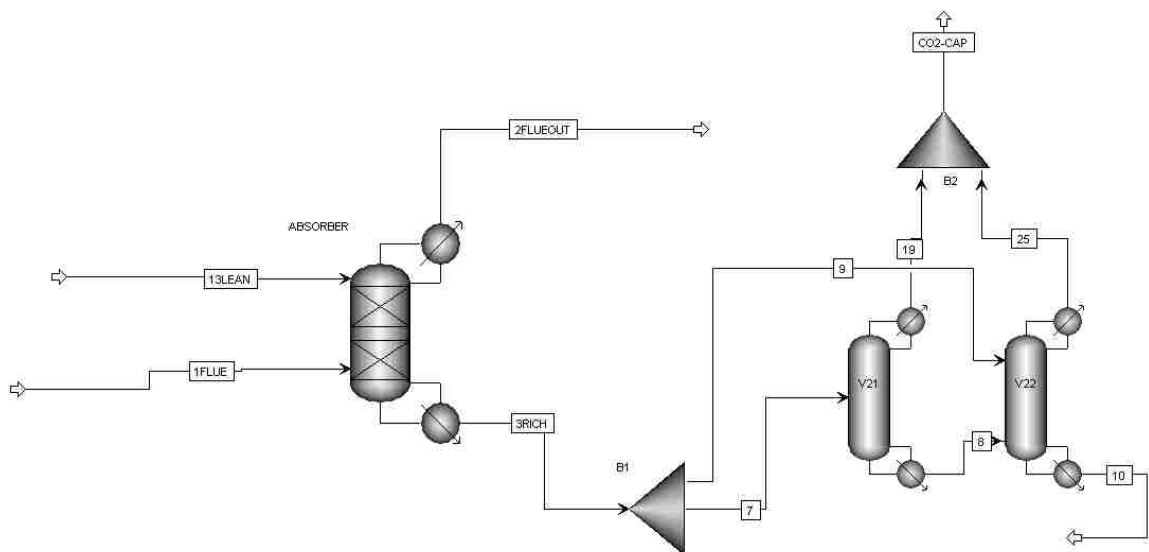


Figure 5.3. Benfield Process Flow Diagram.

Results from using the updated model are shown in Table 5.1. The use of the RGibbs reactor instead of a stoichiometric reactor greatly changes the flue gas composition coming from the PCFB. Since some carbon monoxide is formed, this indicates incomplete combustion being calculated via thermodynamic equilibrium in the reactor. Also, the formation of water is included as opposed to being ignored in the

previous version of the model. While the actual amount of carbon dioxide produced has changed slightly, the capture rate remains around 90% within the Benfield unit. Roughly 40% of the captured carbon dioxide is utilized in the HTSE unit. Since a splitter is used to control the amount of carbon dioxide used in the HTSE, the enriched air generated with the sweep gas remains unchanged. Design specs set in the HTSE maintain the hydrogen to carbon monoxide ratio. Since the combustion chemistry is different using the RGibbs reactor, the converged enriched air composition changed from about 25% oxygen up to around 31% oxygen versus atmospheric 21%.

Without a more rigorous and integrated model that includes the dynamic wind component, estimating overall efficiency is difficult. Table 5.2 displays a comparison of the stand-alone units in the model with other commonly used electric power generating facilities. While SMR efficiency appears low, the innate safety features and reduced construction costs allow SMR technology to be competitive. Wind turbine efficiency is highly dependent upon geographical location, and is an intermittent power source as opposed to base load. The PCFB combustor, while not reaching the efficiency of an ultra-supercritical coal plant, is still effective due to reduced cost and better safety as a PCFB is not dealing with the high temperatures and pressures associated with ultra-supercritical plants.

The levelized cost of electricity measures the rate at which an energy producer must charge in order to break even over the estimated lifetime of the plant. This measure can be used as a base to compare technologies. Table 5.3 contains a select few technologies and their levelized costs based on coming online in 2018 and running for a 30 year lifetime. The idea with the hybrid system is to combine the low cost wind power

with the higher cost coal and nuclear base load capacity power sources. This averaged cost would incorporate renewable energy and lowered carbon emissions.

Table 5.1. Selected Stream Results.

Stream Name	PCFB Flue Gas	CO <sub>2</sub> to HTSE	Enriched Air	Unused CO <sub>2</sub>	Syngas	Coal Air
Total Flow (kmol/hr)	16,390	3,512	5,022	2,154	3,862	14,729
Component Flows (kmol/hr)						
CO <sub>2</sub>	3,902	3,512	-	2,154	178	-
CO	431	-	-	-	1,179	-
N <sub>2</sub>	10,210	-	2,511	-	-	10,180
H <sub>2</sub>	155	-	-	-	2,505	-
O <sub>2</sub>	TRACE	-	2,511	-	-	4,549
H <sub>2</sub> O	1,659	-	-	-	-	-
Mole Fractions						
CO <sub>2</sub>	0.2381	1.0000	-	1.0000	0.0462	-
CO	0.0263	-	-	-	0.3053	-
N <sub>2</sub>	0.6229	-	0.5001	-	-	0.6911
H <sub>2</sub>	0.0095	-	-	-	0.6485	-
O <sub>2</sub>	TRACE	-	0.4999	-	-	0.3089
H <sub>2</sub> O	0.1012	-	-	-	-	-

Table 5.2. Stand-alone Efficiencies.

Individual Efficiencies	
Power Plant Type	Efficiency
PCFB <sup>[4]</sup>	43%
SMR	28%
Wind Turbines <sup>[10]</sup>	34%
Global Average Coal <sup>[11]</sup>	33%
Subcritical coal <sup>[12]</sup>	>38%
Supercritical Coal <sup>[12]</sup>	>42%
Ultra-supercritical coal <sup>[12]</sup>	45-50%

Table 5.3. Levelized Costs of Electricity [10].

U.S. average Total System Levelized Cost	
Technology	2011 \$/MWh
Conventional Coal	100.1
Advanced Coal	123.0
Advanced Coal w/ CSS	135.5
Advanced Nuclear	108.4
Wind	86.6
Solar PV	144.3
Based on new generation resources entering service in 2018	



## 6. FUTURE WORK

To move forward, the current model must be reevaluated. The steam cycles of the SMR, PCFB, and the water required of the HTSE need to be integrated. The syngas product from the HTSE unit must be converted in an electro-catalytic reduction or Fischer-Tropsch reactor to produce chemicals or synthetic fuels. A full exergy analysis should be performed to determine lost work in the hybrid system to further optimize the efficiency.

The entire updated model can then be optimized based on the economic criterion of cost of electricity coupled with chemical production. In order to incorporate the time dependent variable of wind for the wind turbine power generation, the entire model can be updated into Aspen Dynamics, where the entire hybrid energy system can then be optimized once more.

The model can be modified to allow for not only coal as a carbon feedstock, but biomass as well, further increasing the range of applicability of the model. While wind is the initial choice for the intermittent energy source, solar power could also be used, allowing the model to be more applicable geographically as well.

Energy research being conducted at the Missouri University of Science and Technology includes wind turbine analysis, biomass gasification, solar PV work, and SMR modeling. In addition, a laboratory containing a functioning HTSE unit will be useful in comparing updated model outputs with experimental results.

## **II. DYNAMIC PROCESS MODELING OF A SUSTAINABLE COAL, WIND, AND SMALL MODULAR REACTOR HYBRID ENERGY SYSTEM**

### **ABSTRACT**

The proposed coal, wind and nuclear hybrid energy system would combine a renewable energy source, wind, with traditional and stable energy sources, coal and nuclear, to create an integrated and sustainable system. A next generation small modular nuclear reactor will be evaluated (SMR). The coal system will employ a pressurized circulating fluidized bed reactor, which can not only utilize coal, but also use biomass as a carbon feedstock. This system also employs a high temperature steam co-electrolysis unit for efficient utilization of carbon dioxide emissions for the production of synthetic gas that can be used to generate transportation fuels or chemicals.

A rigorous dynamic process model of the system has been constructed. This model will allow for proper scaling of each individual component in the overall hybrid system along with the dynamic characteristics inherent in a fluctuating wind system. Increased integration of the water and heat cycles will be evaluated for improved efficiency. A detailed Aspen Plus user model will be utilized to demonstrate the feasibility of the main hybrid energy system components. Aspen Dynamics modeling will integrate the main process model with the dynamic wind model to look at overall sustainability, power generation, and chemical production.

## 1. INTRODUCTION AND BACKGROUND

As population and economies grow, so does the demand for reliable electricity. Traditionally, this demand was met through combustion of carbon based fuels. This approach has resulted in increased concentrations of carbon dioxide in the atmosphere. New techniques for power generation are being considered, such as electricity produced from renewable sources. Where combustion can be controlled through operation, most renewable energy sources are highly dynamic in nature and pose a significant challenge to providing reliable energy that meets variable demand. In the case of wind power, wind velocity determines power generation, which can vary considerably based on time of day, location, and season. Figure 1.1 shows how much variation is possible at a single site month to month over several years of operation.

Production variability must be coupled with either energy storage or a secondary, fast acting generator such as a gas combustion turbine in order to better match the load profile. The proposed hybrid system consisting of a small modular nuclear reactor (SMR) and pressurized circulating fluidized bed (PCFB) combustor for stable, base load type power generation coupled with the dynamic wind generation alongside carbon dioxide utilization via high temperature steam co-electrolysis handles the issues of dynamic power generation and carbon dioxide emissions. The main idea behind the proposed system is to generate electrical power using a carbon based fuel that produces carbon dioxide which will be utilized with high temperature steam generated from the SMR to produce syngas (hydrogen and carbon monoxide gases) when power is available, capturing the excess wind energy and storing it in chemical form.

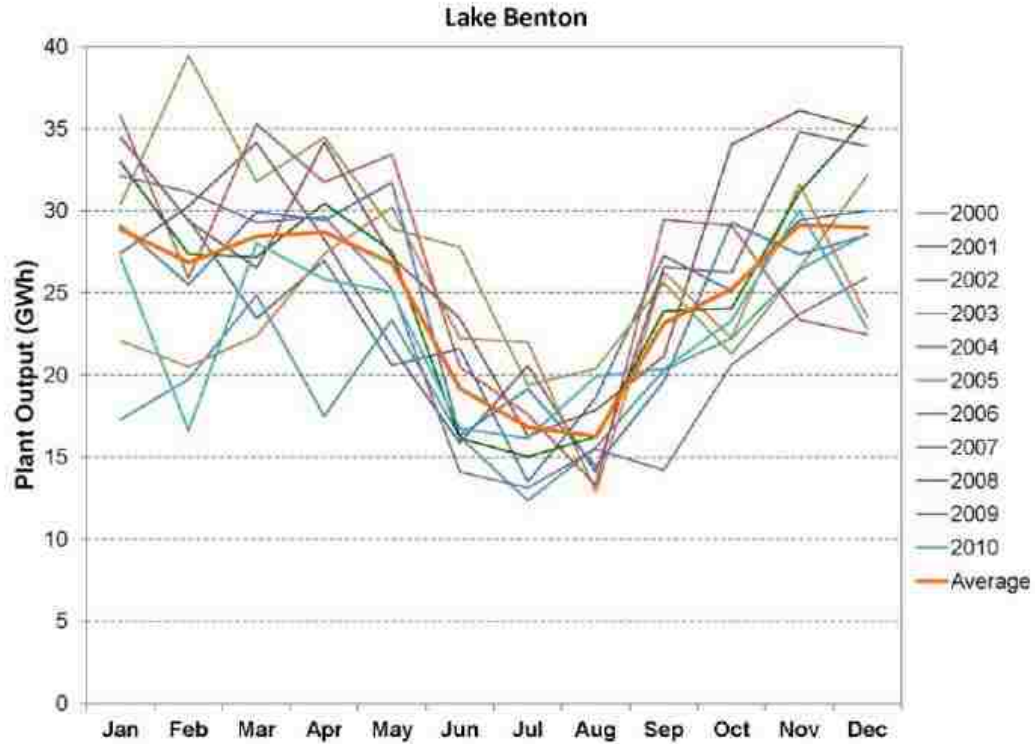


Figure 1.1. Monthly Wind Energy Production [13].

The current work utilizes the results of a steady state Aspen Plus simulation of the PCFB and SMR base load producers, the carbon dioxide separation unit, and the co-electrolysis unit. This work expands upon the results by simplifying the steady state models and exporting them into a model using Aspen Plus Dynamics, where the wind power generation is introduced together with grid demand, and dynamic production of syngas is evaluated.

## 2. METHODOLOGY

The process flow diagram consists of the existing steady state simulation of the base load power generation from the nuclear SMR and coal PCFB linked through the high temperature steam electrolysis (HTSE) unit (Figure 2.1). Coal is first combusted in the PCFB and the effluent sent to the carbon dioxide separation and capture unit. From there, captured carbon dioxide and steam from the SMR are combined with sweep gas (air) in the HTSE, generating syngas and an oxygen enriched air stream. This oxygen enriched air stream is then combined with makeup air and fed to the PCFB to support oxygen enriched combustion.

The PCFB reactor was modeled after the performance of the Alstom P200 operating in Europe [9] (Figure 2.2). The model uses two parallel operating systems where coal has been reconciled into a material stream consisting of molecules based on the ultimate analysis. It is then combined with enriched air and sent to an RGIBBS reactor in Aspen Plus, which calculates reaction products based on thermodynamic equilibrium. The energy generated in this block is used to heat water to produce steam and generate electricity through a steam turbine. The effluent from the reactor goes through a second turbine to capture additional energy before it is sent out of the PCFB hierarchy. The steam cycle generates roughly 80 MW<sub>e</sub> while the effluent turbine captures around 20 MW<sub>e</sub>, bringing the entire PCFB generation to 200 MW<sub>e</sub>.

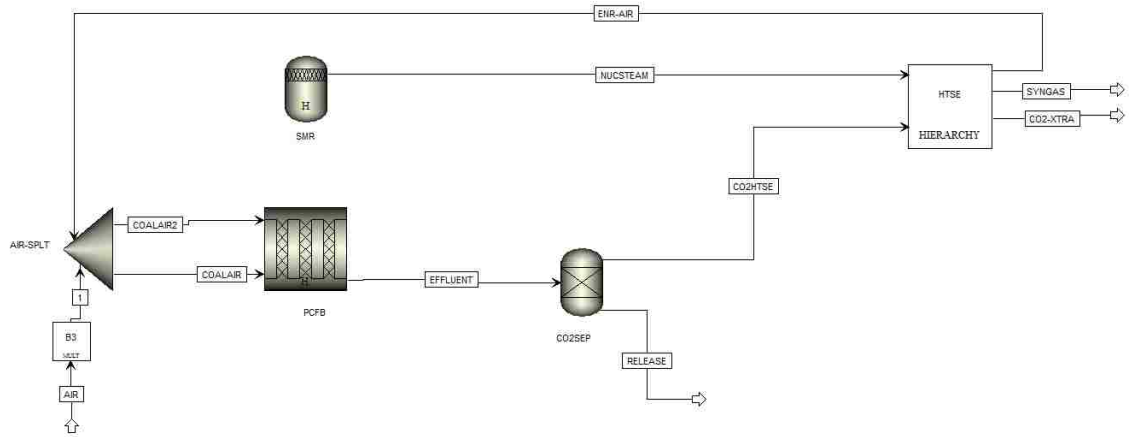


Figure 2.1. Steady State Model.

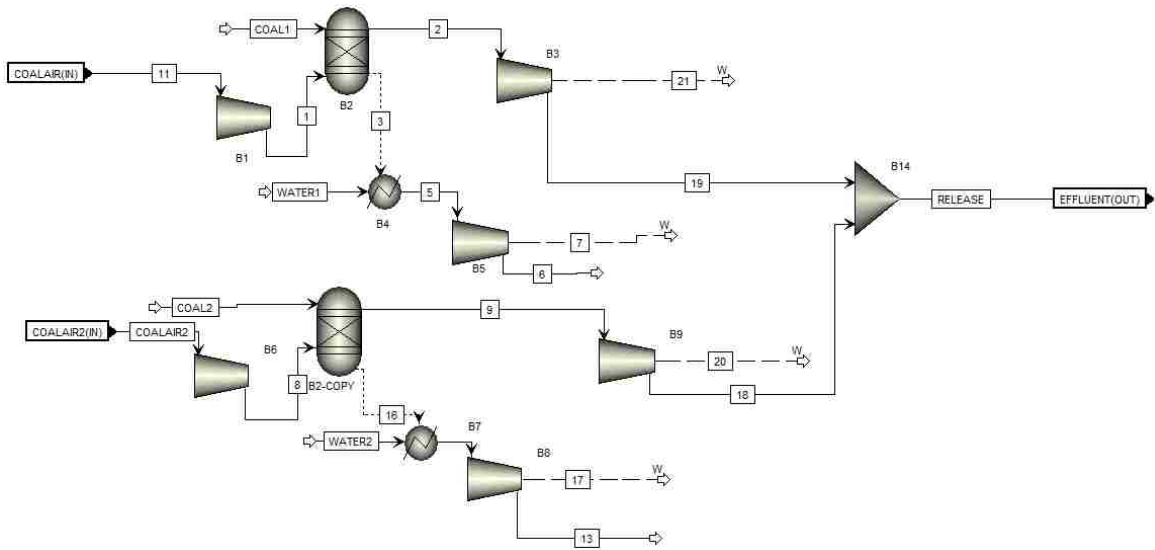


Figure 2.2. PCFB Hierarchy.

The flue gasses from the PCFB are sent to a carbon dioxide capture unit based on the Benfield process (Figure 2.3). The flue gasses are sent into an absorber containing aqueous potassium carbonate supported with piperazine. The carbon dioxide is absorbed into the aqueous phase then sent into a double matrix stripper to generate a pure stream of carbon dioxide, capturing nearly 90% of the carbon dioxide produced [7].

The nuclear SMR model is based on the Westinghouse design considerations. The Aspen Plus model representation of the Westinghouse design is shown in Figure 2.4. A heat stream is used to simulate the  $800 \text{ MW}_t$  being given from the nuclear core. The heat is transferred to an internal water cycle that is present in the SMR design. This internal water cycle then transfers heat to an external steam cycle that generates the  $225 \text{ MW}_e$  [5, 6]. The exhaust steam is then sent to be utilized in the HTSE.

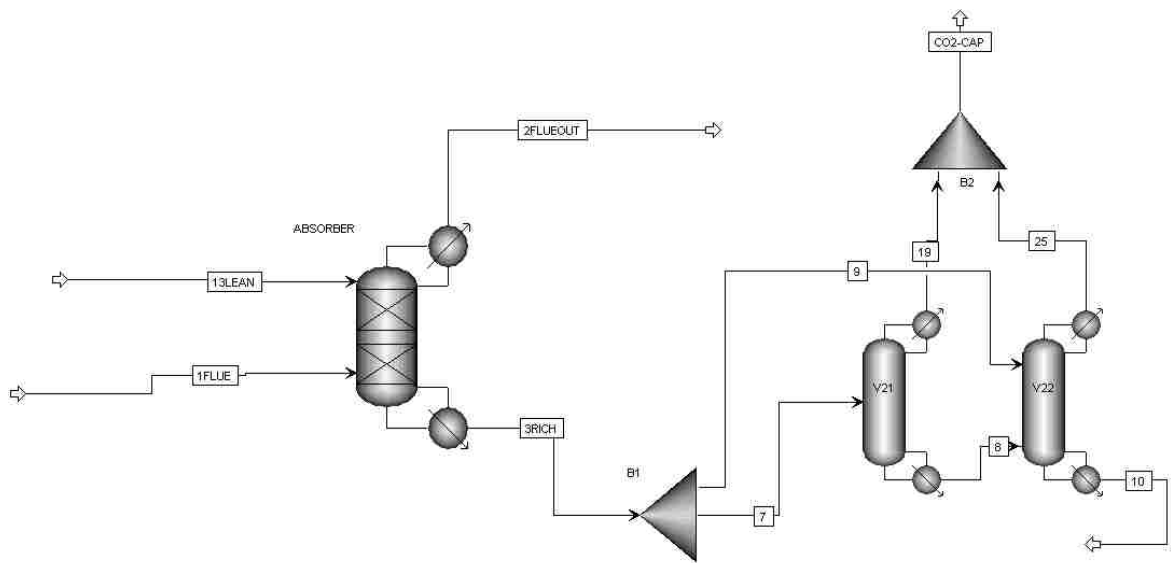


Figure 2.3. Carbon Dioxide Capture.

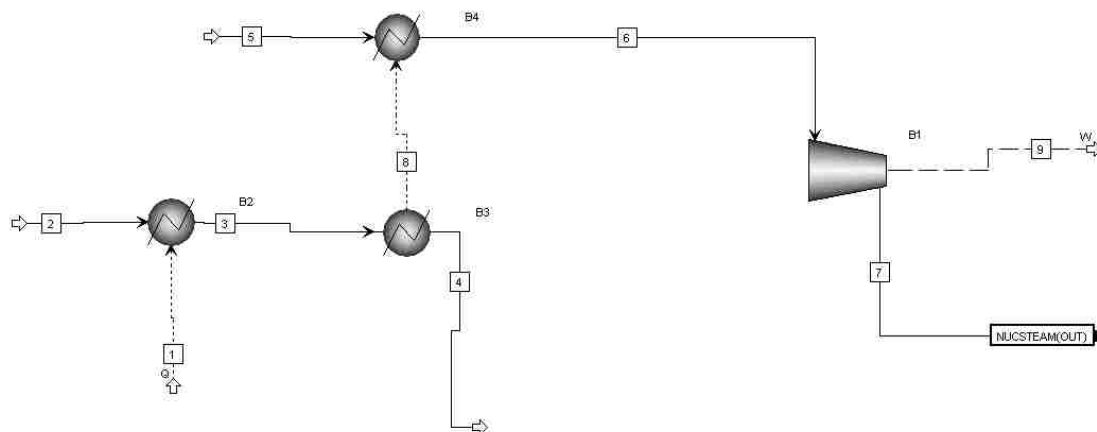


Figure 2.4. Nuclear Small Modular Reactor.

The High Temperature Steam Electrolysis model used was developed by Idaho National Labs. The model is prepared in multiple hierarchies. The outer hierarchy (Figure 2.5) handles the inlet and exit components. It takes the captured carbon dioxide and steam, pressurizes the gases, mixes and heats the components with recycled gases before being sent into the inner hierarchy. It also pressurizes and heats the air sweep gas that carries the oxygen product from the electrolysis reaction. The inner hierarchy (Figure 2.6) handles the reactions to produce syngas. The first reactor models the gas shift reaction in an RGibbs reactor. The products are then sent to an RStoic reactor to model the water and carbon dioxide electrolysis reactions. The gasses are sent to a Sep block to remove the oxygen produced which is carried out by the air sweep gas. The final reactor block is a second gas shift RGibbs reactor. The reactors are controlled by in-line FORTRAN design-specs set up in Aspen Plus. The in-line code modifies flow rates, temperatures, and syngas production controlled by a co-electrolysis model based on number of theoretical cells present in the unit [8].



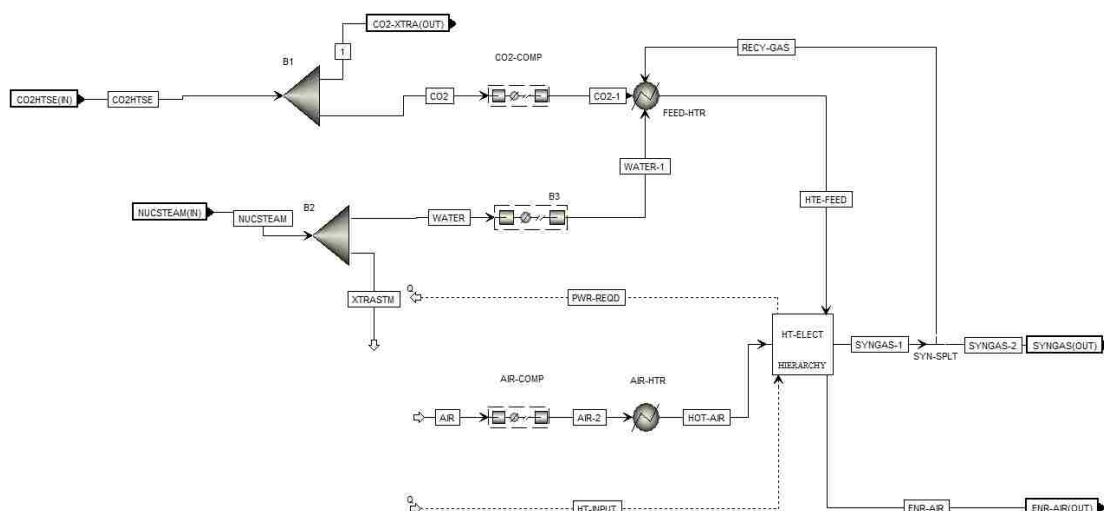


Figure 2.5. High Temperature Steam Electrolysis, Outer Hierarchy.

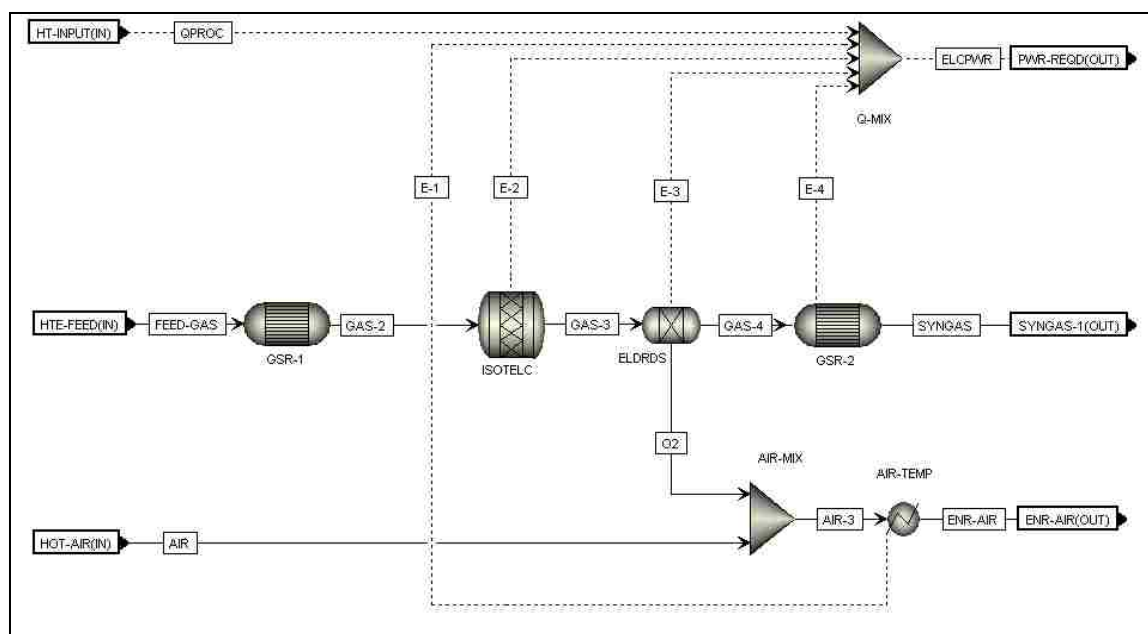


Figure 2.6. High Temperature Steam Electrolysis, Inner Hierarchy.

To incorporate the dynamic wind model with the steady state base load power generators, several simplifications had to be made to the Aspen Plus model before

exporting to Aspen Dynamics. One major assumption made is the base load generators will operate at steady state conditions. The purpose of the dynamic model is to monitor the interaction of dynamic wind with the production of syngas, not any upset condition faced by the PCFB or SMR.

Since the dynamic model is only concerned with the final products from the PCFB, the effluent streams and energy produced through the turbines can be reconciled and treated as steady products (Figure 2.7). The effluent streams from the parallel units are mixed and sent to the carbon dioxide capture unit. The power generated from the steam cycle turbines and the exhaust gas turbines is mixed and made available for use.

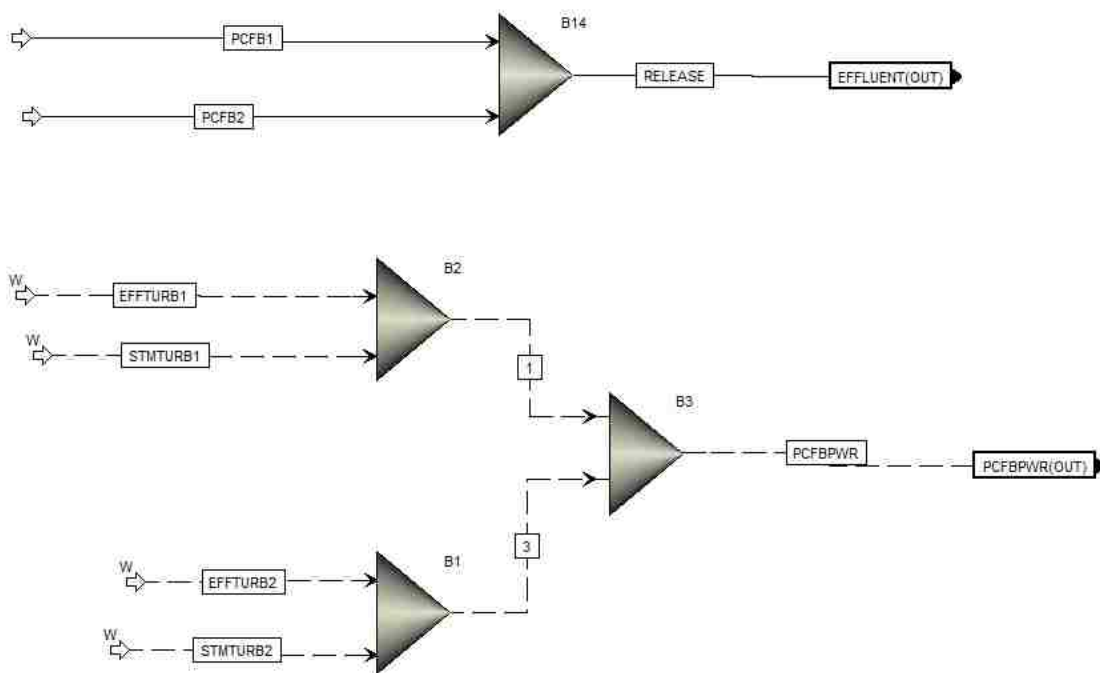


Figure 2.7. Reconciled PCFB.

The carbon dioxide capture unit's complex absorption models do not need to be run in the dynamic case. The final product stream from the unit is reconciled and its

information is used to model a Sep block to separate the carbon dioxide from the PCFB effluent. The Sep block completely replaces the carbon dioxide capture unit hierarchy.

The High Temperature Steam Electrolysis hierarchy required a large number of simplifications and modifications in order to be exported into Aspen Dynamics. The largest change comes in the removal of the in line FORTRAN code written for the design specs as they are not supported in Aspen Dynamics. Reconciliation of streams is not possible as syngas production had to be modeled dynamically as it changed with varying power available. Multiple steady state calculations were run varying the number of theoretical cells present in the unit and recording the power required, inlet flow rate of chemical species, and syngas production. This information was used to create an RStoic reactor capable of producing the same syngas based on the amount of reactants fed (Figure 2.8).

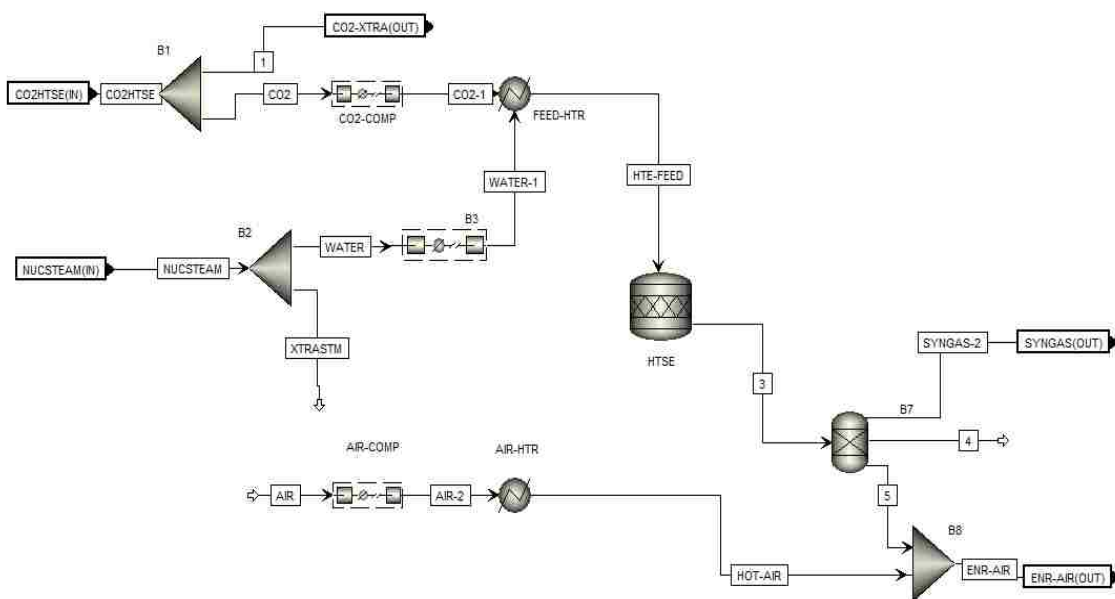


Figure 2.8. Simplified High Temperature Steam Electrolysis.

Due to the reconciliation of the streams in the PCFB, the recycled enriched air stream no longer needs to be fed to the PCFB thus removing a tear stream which improves the simulation run time and convergence rate. With these simplifications, the Aspen Plus model was capable of being exported as a flow driven simulation into Aspen Dynamics.

With the simulation exported into Aspen Dynamics, the wind power generation was implemented and grid electrical demand was evaluated (Figure 2.9). A Pseudo-Random Binary Signal was used to simulate the random generation of wind power. The PRBS varies power generated between 0 and 100 MW<sub>e</sub> on a period of 5 minutes. Grid demand was simulated with a sine wave signal starting at 200 MW<sub>e</sub> with 200 MW<sub>e</sub> amplitude over a period of 24 hours. This allowed an example simulation of 12 hours where grid demand started at a base level, increased over the course of a day to peak demand, then diminished. The power generated from the PCFB, SMR, and wind along with grid demand was fed to a mixer block. With power generated and grid demand in opposite magnitudes, what remained after the mixer was either excess power or a power deficit. If excess power was available, it was then fed to the HTSE to allow syngas production.

The HTSE does not directly use the remaining power after grid demand has been met. A series of controllers were implemented to modify the flow of components into the stoichiometric reactor (Figure 2.10). These controllers used the information gathered from the multiple steady state simulations that varied the number of cells available in the HTSE to modify the flow splitting blocks to feed the correct amount of components to the stoichiometric reactor.

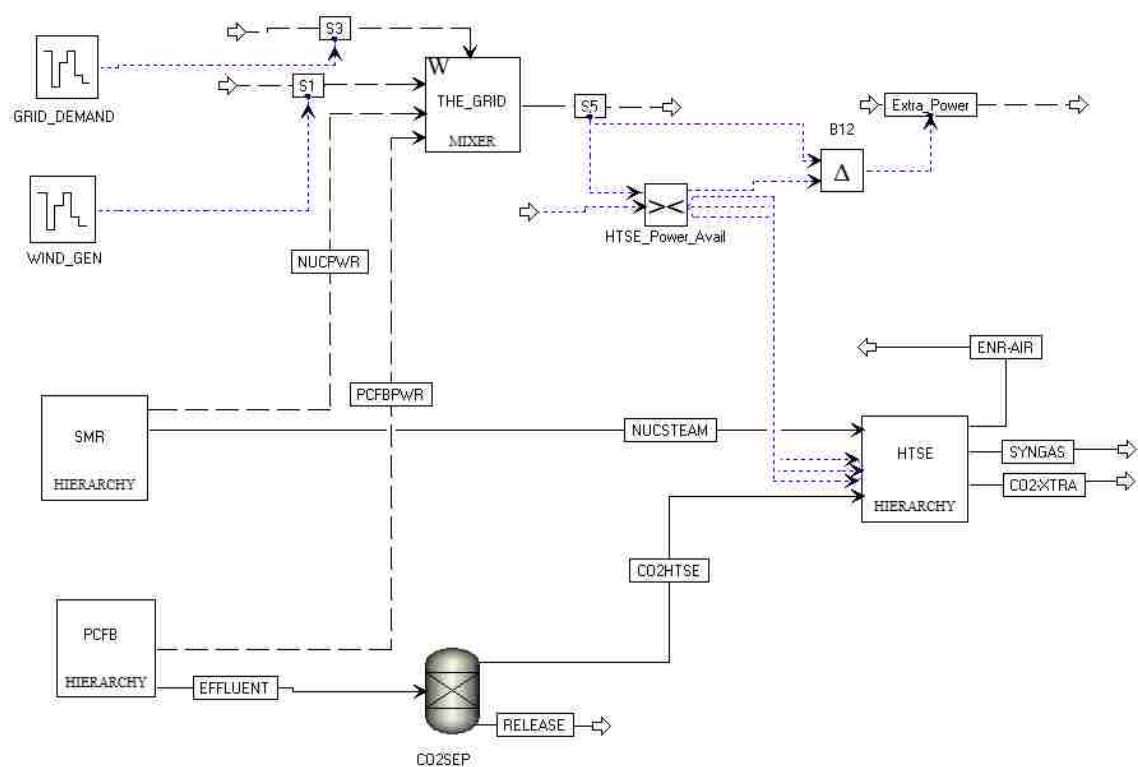


Figure 2.9. Dynamic Overall Hybrid Energy System.

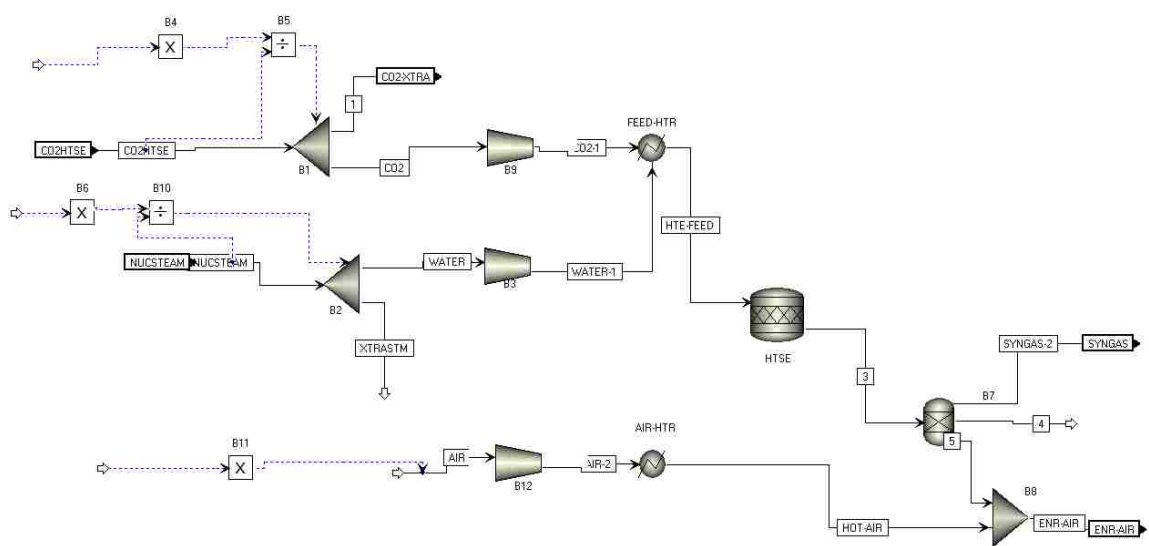
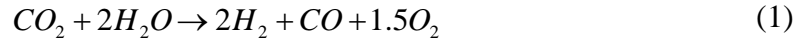


Figure 2.10. Dynamic High Temperature Steam Electrolysis Hierarchy.

### 3. RESULTS

In the presented model, the HTSE required 252.71 MW<sub>e</sub> running at full capacity at steady state. To get the HTSE to run dynamically, steady state solutions were recorded at various intervals in order to generate performance curves related to power consumption. Conversion data of carbon dioxide and steam was used to generate the parameters used in the stoichiometric reactor (Table 3.1). The conversion rates do not vary much over the range simulated so an average conversion rate was used in the stoichiometric model along with the following equations:



The parameters used in the controllers for the HTSE were derived from the steady state inlet flows of reactants to the HTSE at various intervals (Table 3.2). These values were regressed to create an operating curve. A linear relationship and the equations obtained relating power used by the HTSE to the flow rate of the respective reactant were calculated (Figure 3.1).

Grid demand was modeled to mimic a single half day ramping up from a base level to peak demand then back to the base over 12 hours (Figure 3.2). The power generated changes randomly in magnitude from a base 50 MW<sub>e</sub> up to an amplitude of 50 MW<sub>e</sub> on a five minute interval (Figure 3.3).

The final result stemming from the combination of base load power generation of the coal PCFB and nuclear SMR coupled with the dynamic wind turbines meeting grid electrical demand lead to the available power to run the HTSE and produce syngas. At the beginning time 0, production is steady at a maximum value (Figure 3.4). As time

progressed, syngas production declined as grid demand increased. Instead of following an inverse of the sine wave generated from grid demand, the amount of syngas produced fluctuated representing the utilization of the dynamic wind power generated. In conclusion, the steady state Aspen Plus model reconciliations and simplifications were exported into Aspen Dynamics and are capable of incorporating grid demand and dynamic wind fluctuations to produce syngas.

Table 3.1. High Temperature Steam Electrolysis Conversion.

Power Required (KW)	Conversion	
	CO <sub>2</sub> -> CO	H <sub>2</sub> O -> H <sub>2</sub>
-252710	0.870507234	0.9180005
-227460	0.86892906	0.9172446
-202200	0.869661788	0.9176403
-176920	0.870424096	0.9180224
-151620	0.870014239	0.9177206
-126360	0.868938465	0.9172312
-101090	0.869330611	0.9174215
-75816	0.870467966	0.9180019
-50544	0.869104118	0.9173079
-25272	0.869236337	0.9173749
-12633	0.869237747	0.9173124
Average Conversion	0.869622878	0.9175707

Table 3.2. High Temperature Steam Electrolysis Reactants.

	Steam	CO2	HTSE.AIR		
Power Required	Steam	CO2	O2	Total	N2
(KW)	(lbmol/hr)	(lbmol/hr)	(lbmol/hr)	(lbmol/hr)	(lbmol/hr)
-252710	5976.362	2967.1696	1461.2836	6958.4933	5497.2097
-227460	5375.6901	2683.1058	1315.1526	6262.6316	4947.479
-202200	4774.5056	2384.9744	1169.0273	5566.7967	4397.7694
-176920	4176.82	2084.1676	1022.9234	4871.064	3848.1406
-151620	3589.538	1778.5902	876.7771	4175.1292	3298.3521
-126360	2988.3553	1488.703	730.6409	3479.2423	2748.6014
-101090	2390.7866	1189.8173	584.516	2783.4095	2198.8935
-75816	1791.8959	891.2444	438.3852	2087.5485	1649.1633
-50544	1195.5646	595.0615	292.2608	1391.7183	1099.4575
-25272	597.7823	297.4519	146.133	695.8715	549.7385
-12633	298.8912	148.5964	73.0425	347.8213	274.7788

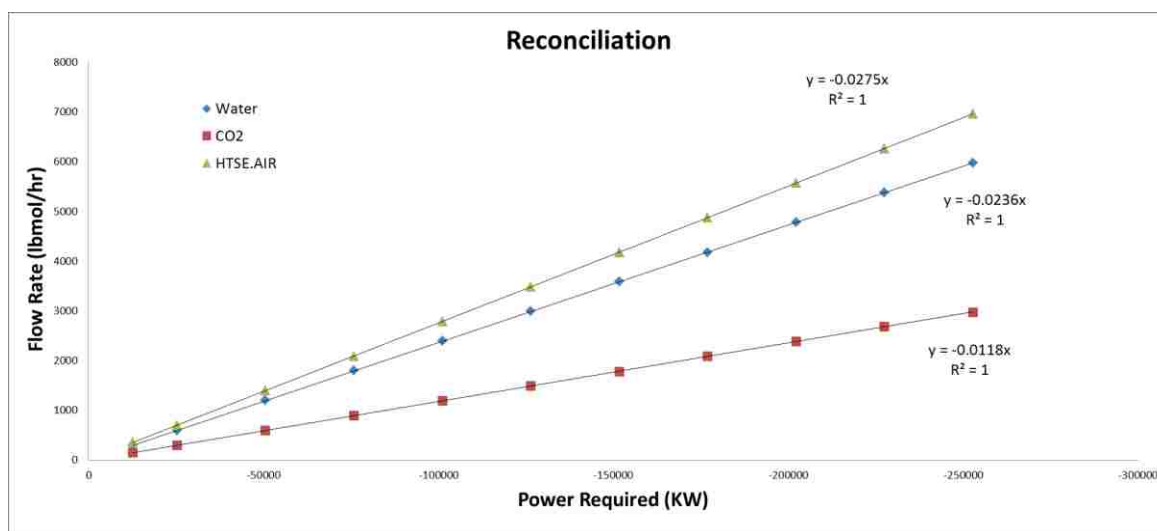


Figure 3.1. Operating Curve for HTSE Reactants.



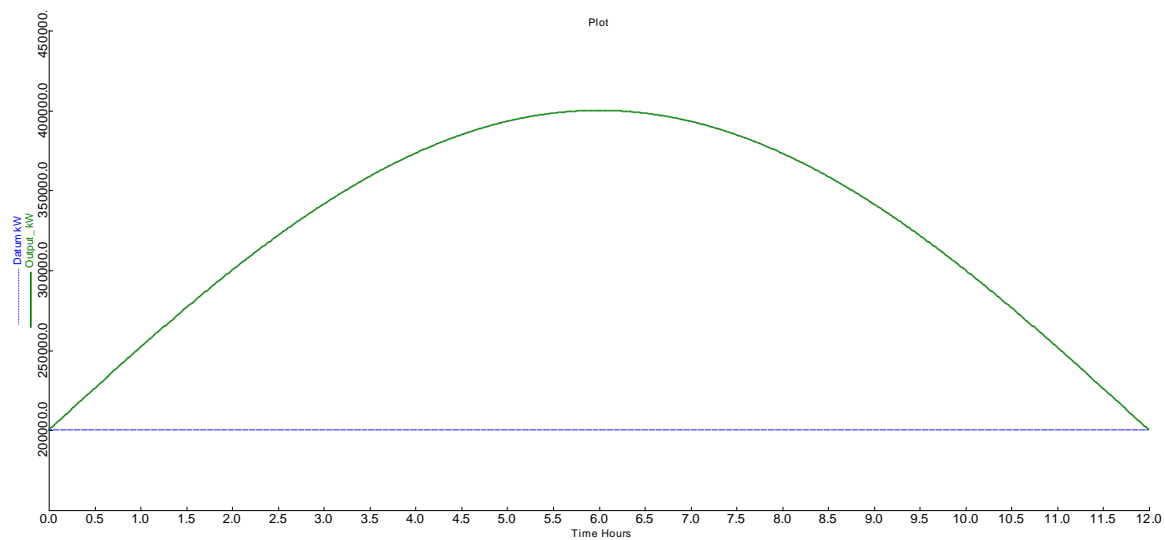


Figure 3.2. Grid Demand.

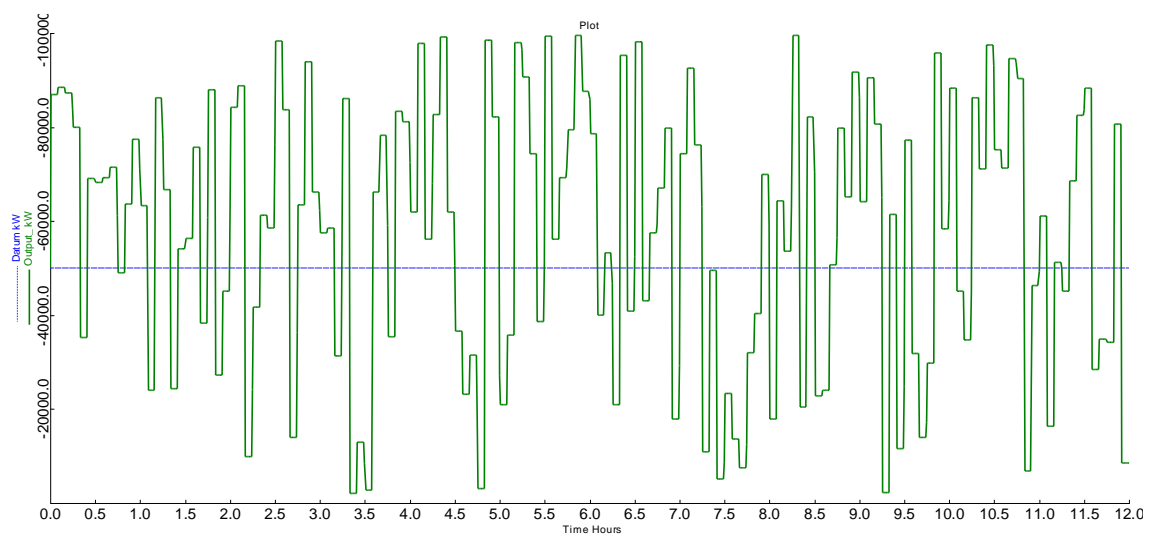


Figure 3.3. Dynamic Wind Power Generated.

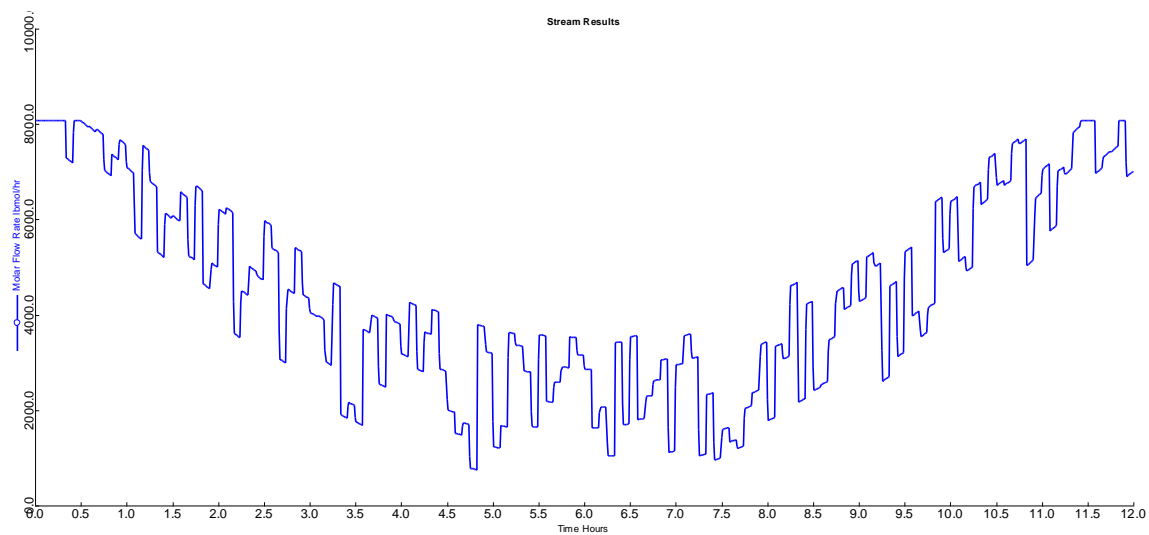


Figure 3.4. Dynamic Syngas Production.

#### **4. FUTURE WORK**

The dynamic model used in this work only considered a randomly generated wind profile along with a simple grid demand over 12 hours. With this model in place, future work will involve a full year simulation in order to generate potential syngas production capabilities. Real wind data will be used in place of a random source to improve model realism and accuracy. Real grid data will also be obtained to match true demand over full day and night cycles as well as seasonal demand changes. With real data implemented in the dynamic model, optimization can be performed based on cost of electricity combined with sale of chemicals, allowing for scaling up and down of the various power generation sources. Potential changes could also include how much carbon dioxide to capture and utilize along with the size of the HTSE unit. The addition of a possible carbon tax will also be evaluated. The optimized dynamic model will then be used to generate a production possibilities frontier showing possible production rates of electrical power versus chemicals produced.

### **III. PRODUCTION POSSIBILITIES OF A SUSTAINABLE COAL, WIND, AND SMALL MODULAR REACTOR HYBRID ENERGY SYSTEM**

#### **ABSTRACT**

The availability of cheap electricity is one of the biggest factors for improving quality of life. With the debate on the effects of carbon dioxide emissions continuing, several countries have either implemented or are considering the reduction of emissions through various economic means. The push for large-scale renewable sources of energy has met problems with regards to energy storage and availability. The proposed coal, wind, and nuclear hybrid energy system would combine a renewable energy source with traditional and stable energy sources to create an integrated and sustainable system. A next generation small modular nuclear reactor will be evaluated. The coal system will use a pressurized circulating fluidized bed system, which can not only take coal, but also biomass as a carbon feedstock. This system also employs a high temperature steam co-electrolysis unit for the utilization of carbon dioxide emissions for the production of synthetic gas which can be used in the production of transportation fuels or chemicals.

An existing rigorous dynamic process model was used to simulate the potential output of the system based on real world dynamic data. System inputs included a full year of dynamic wind speeds for variable power generation and simulated electrical grid demand. These inputs varied the amount of power available for synthetic gas production, and thus theoretical production possibilities for the hybrid system over a year of operation were formed. This information was used to determine overall process economics by comparison to a conventional coal system by using the sale of synthetic gas

and levelized cost of electricity. It was determined that a syngas sale price as low as \$0.33 per 1,000 SCF allowed for certain hybrid systems to be competitive with conventional technologies.

## 1. INTRODUCTION AND BACKGROUND

Since the industrial revolution, fossil fuels have been combusted to power mankind's machines in the effort to do work. While these machines have benefited society greatly, a debate has arisen to determine whether or not the carbon dioxide emitted from the combustion of these fossil fuels is having a negative effect on the Earth's atmosphere. Carbon neutral or carbon free sources of renewable power are being explored such as wind and solar. One of the major issues with these renewable energy sources is their inherently dynamic nature [14].

Wind turbines generate power when the wind has enough velocity to turn the blades on the turbine yet low enough so as to not damage the unit. Wind generation depends greatly on the time of day, time of year, and climate of the area in order to generate power. The demand for reliable, instant, and cheap electricity does not follow with these variable wind speeds. Base load power generation in the form of combusting carbon resources has been the norm since it can be controlled to match energy demanded. Nuclear power has a similar capability.

One way to handle the dynamic behavior of renewables is through storage. Several methods for storage exist such as batteries, pumped-storage hydroelectricity, and molten salts. The proposed hybrid energy system utilizes a form of chemical storage. The hybrid system consists of a pressurized circulating fluidized bed (PCFB) coal combustor alongside a small modular nuclear reactor (SMR) that provides base load electricity. Wind turbines are also used as a source of renewable energy. A high temperature steam co-electrolysis (HTSE) unit is coupled with this system. The HTSE unit is capable of consuming the carbon dioxide that is generated from coal combustion

alongside the steam generated from the SMR. This HTSE unit will run when power generated exceeds demand and generate a combination of carbon monoxide and hydrogen known as syngas. This method of chemical power storage allows the hybrid system to utilize the carbon dioxide produced from base load power generation while handling the intermittent energy produced from the renewable wind resource.

The current work utilizes an existing Aspen Dynamics model that is capable of simulating the production characteristics of the PCFB, SMR, wind, and HTSE unit. This work runs a full year simulation using real world wind and electricity demand data in order to capture the production possibilities of the hybrid energy system. The production results were then compared to a conventional coal base load generator with wind power to determine economic viability.

## 2. METHODOLOGY

The existing Aspen Dynamics model consists of five key areas: PCFB model hierarchy, SMR model hierarchy, wind model, grid demand model, and the HTSE hierarchy. The dynamic model is flow driven and was imported from a steady state Aspen Plus simulation. The steady state PCFB model was based on an existing coal plant operated by SARGAS [9]. The model utilizes equilibrium reactions in order to determine heats of combustion and reaction products. This model was simulated and consolidated to maintain combustion products and electricity produced before it was exported into Aspen Dynamics. The steady state SMR model was constructed using thermal and electrical output data from Westinghouse [5]. The SMR model simulates the heat from the nuclear reactor and transfers it through an inner and outer heat exchanger loop to generate steam and then electricity through a turbine. The steady state HTSE model used was first developed by Idaho National Laboratory [8] before being modified for use on an industrial scale. This HTSE model was consolidated using stoichiometric reactions in place of design specifications and in-line Fortran programming before being exported into Aspen Dynamics.

The wind model was handled directly in Aspen Dynamics. Wind turbines have a range of wind speeds wherein they will generate electricity. The Vestas V90 wind turbine was chosen for this work [15]. The Vestas V90 is a 3.0 MW rated wind turbine with a cut-in wind speed of 3.5 meters per second and a cut-out wind speed of 25 meters per second along with a unique power curve. This power curve represents how much electricity will be generated based on the wind speed.



The existing Aspen Dynamics model was designed for a twelve hour sample simulation using a random number generator for wind speeds and a sine function for grid demand. In order to determine real world performance of the system, wind speed data and grid demand data was used in the dynamic model. Wind speed data was acquired from the National Wind Technology Center [16]. The center hosts wind statistics for a number of years. For this work, one minute data of wind speeds at 80 meters was selected from the year 2013 (Figure 2.1). Grid demand data was gathered from Southwest Power Pool (SPP) [17]. SPP provides grid load and forecast data taken every five minutes. Values from the year 2013 were used in this work (Figure 2.2).

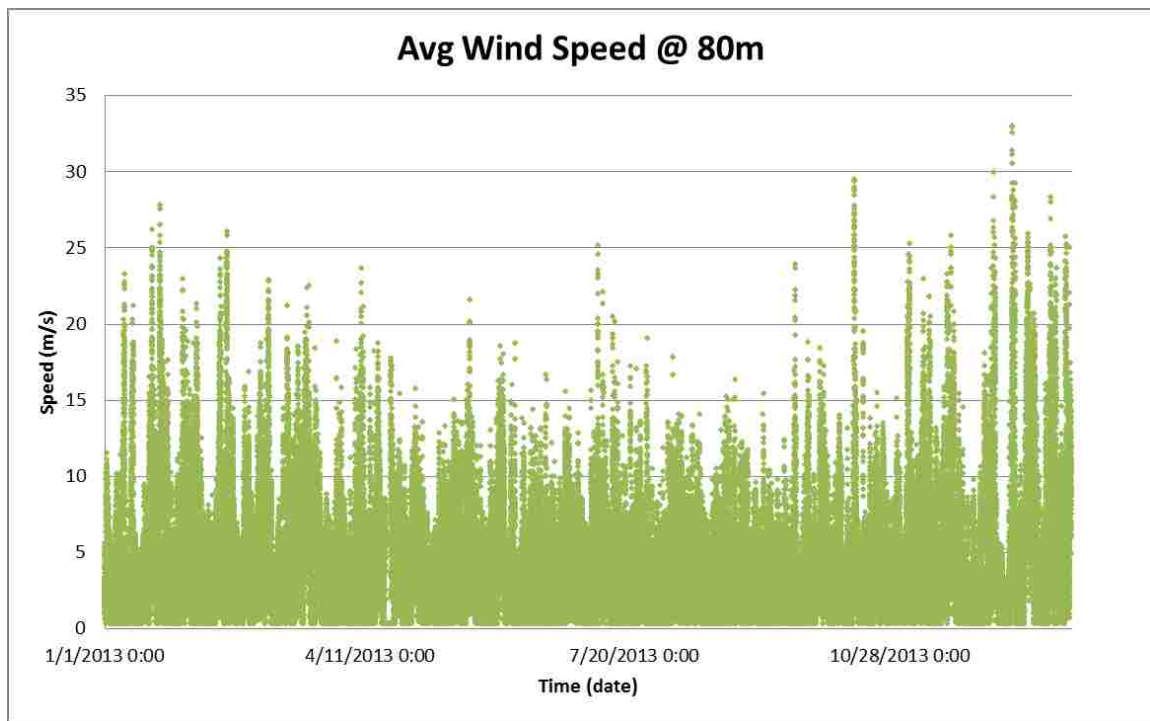


Figure 2.1. Average Wind Speeds from National Wind Technology Center.

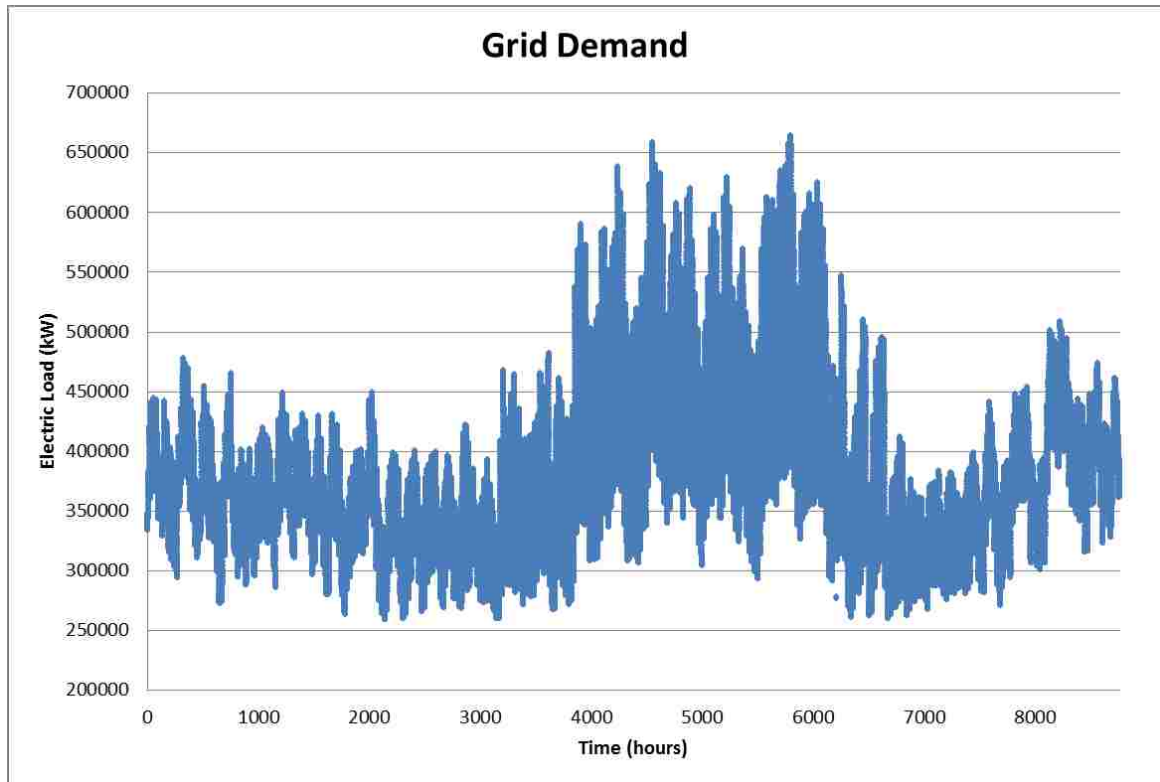


Figure 2.2. Scaled Grid Demand from Southwest Power Pool.

The real grid demand data was for SPP's entire service area. This data was scaled down into a 258 – 663 MW range to be used on a similar level as the dynamic model 411 MW base load plus 120 MW dynamic wind capacity. This range was calculated so that at the minimum demand, the maximum capacity of the hybrid system could be fully utilized in the HTSE scale model. The wind measurements were used every five minutes instead of every minute in order to match the number of data points from the grid demand.

The dynamic wind model applies the Vestas V90 power curve to the wind speed data to generate a signal. This signal is then multiplied by the number of turbines in the model. The signal is then converted in order to maintain unit compatibility. The model

signal then modulates an Aspen Dynamics work stream to simulate the electricity generated from the wind turbines (Figure 2.3). The scaled grid demand signal is multiplied by a similar conversion factor before modulating another work stream. The wind power and grid demand work streams are fed into a mixer alongside the base load SMR and PCFB work streams to determine if there is any power available for the HTSE. The resulting work stream from the mixer is then measured and the information is sent through a control signal in order to regulate the flow of reactants entering the HTSE to produce syngas. In the event that grid demand exceeds power generated, the information is recorded and handled as peak demand that needs to be compensated for later. Figure 2.4 displays the modified model with the real world grid demand and wind turbine models implemented.

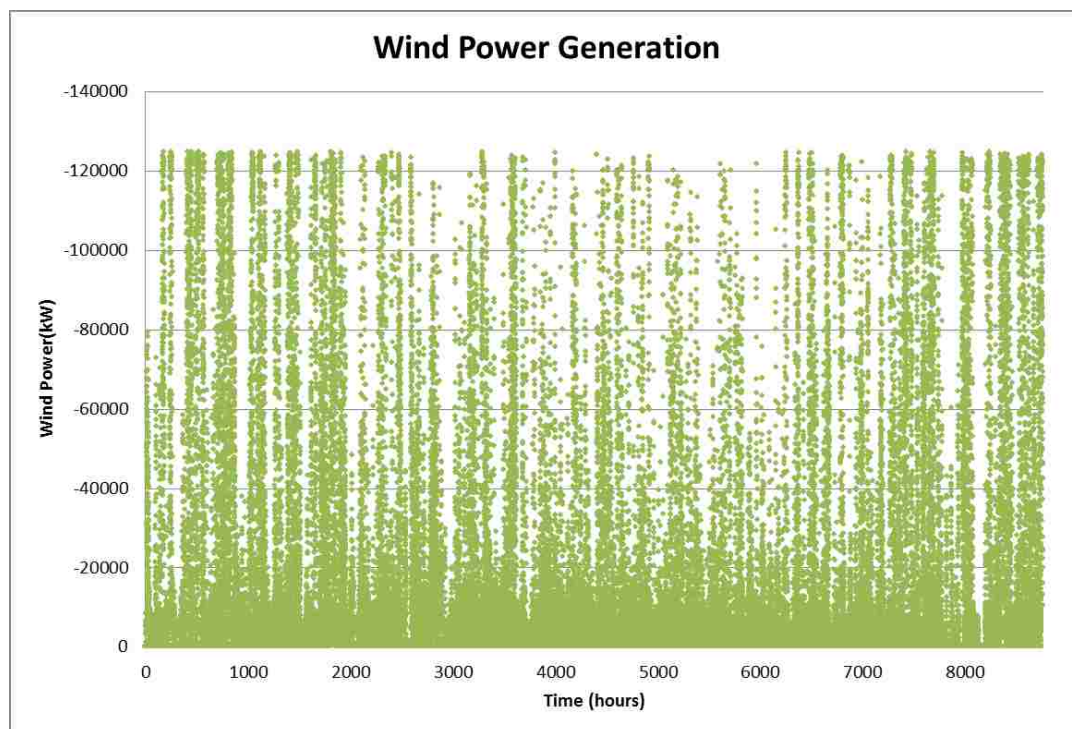


Figure 2.3. Wind Turbine Model Power Generated.

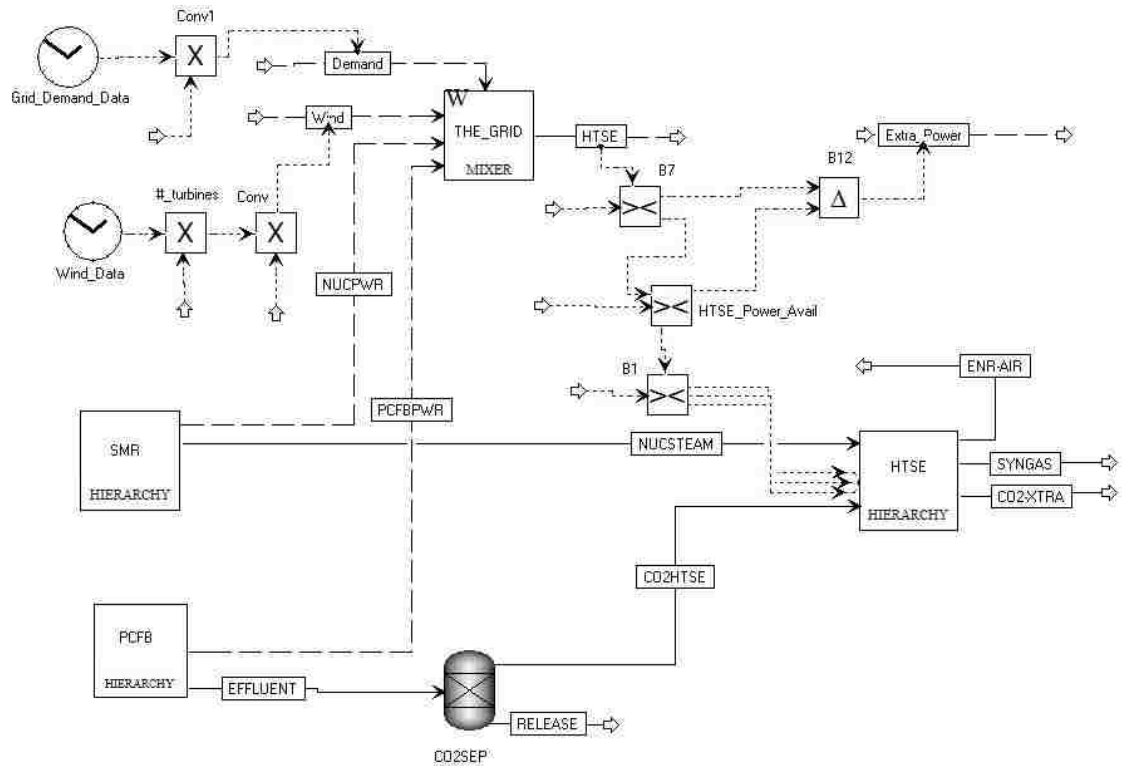


Figure 2.4. Real Data Modified Process Flow Diagram of Aspen Dynamics Model.

Due to constraints on the number of data points able to be used in Aspen Dynamics Timedata models the simulation was split into twelve segments each simulating one month. The base hybrid energy system consists of two PCFB units each generating  $100 \text{ MW}_e$ , a single SMR unit generating a net  $211 \text{ MW}_e$ , and 40 wind turbines rated at a combined  $120 \text{ MW}_e$ . In an effort to quantify the effect the number of each type of unit has on the hybrid system, multiple systems were modeled and simulated (Table 2.1).

Table 2.1. Hybrid Systems Evaluated.

Power Generating Source				
		PCFB	SMR	Wind
Base System	Number of Units	2	1	40
	Power Produced (MW <sub>e</sub> )	200	211	120
-50% Coal	Number of Units	1	1	40
	Power Produced (MW <sub>e</sub> )	100	211	120
+50% Coal	Number of Units	3	1	40
	Power Produced (MW <sub>e</sub> )	300	211	120
Double Nuclear	Number of Units	2	2	40
	Power Produced (MW <sub>e</sub> )	200	422	120
-50% Wind	Number of Units	2	1	20
	Power Produced (MW <sub>e</sub> )	200	211	60
+50% Wind	Number of Units	2	1	60
	Power Produced (MW <sub>e</sub> )	200	211	180

### 3. SIMULATION RESULTS

The current version of the dynamic hybrid energy system model determines if the electricity generated is greater than the grid demand. The HTSE model is run when there is a surplus of power, reducing carbon dioxide emitted and generating syngas. When there is a power deficit, a peak power generator must be used. A combined plot showing grid demand with power generated is shown in Figure 3.1. In this figure, there are times throughout the simulated year that the hybrid system both exceeds and falls under grid demand.

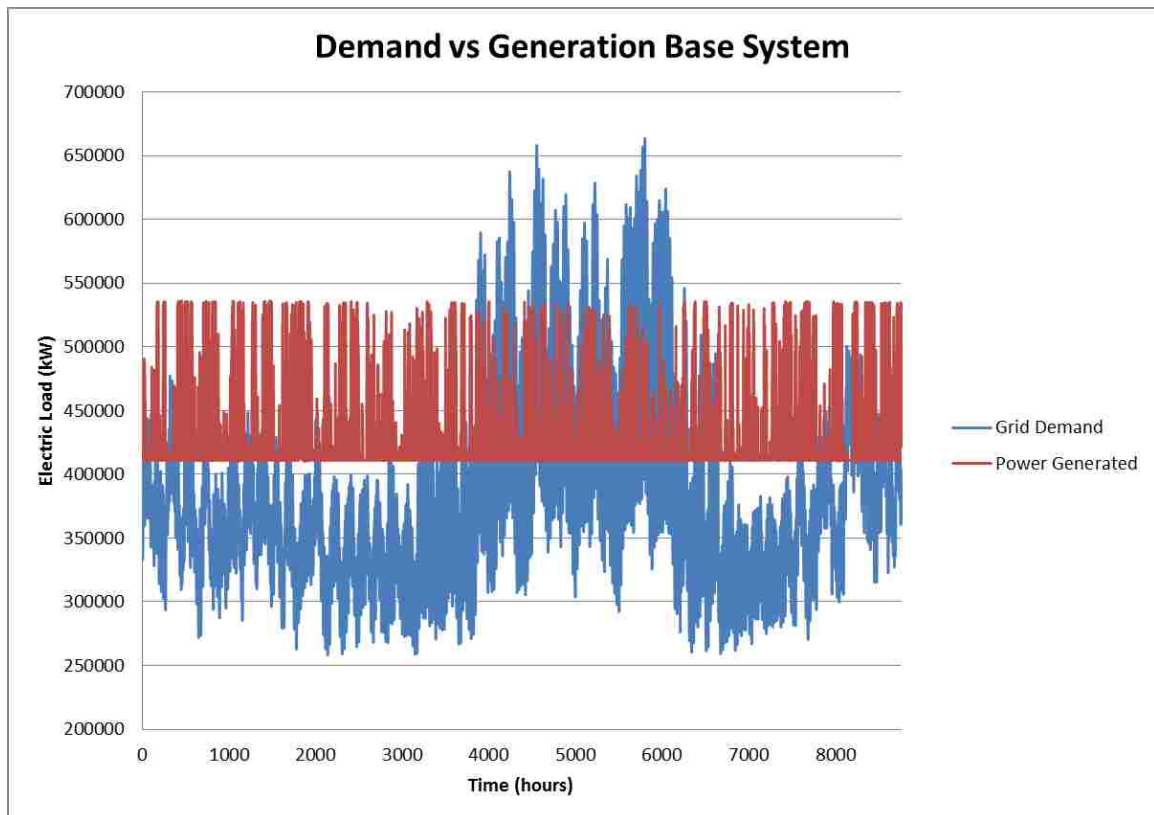


Figure 3.1. Power Generated vs. Grid Demand for Base System.

Peak power demand that must be met with an additional generator is shown in Figure 3.2. From the figure, peak power demand occurs throughout the year as a result of day and night cycles, seasons, and fluctuating wind power. The largest amount of peak power demand occurs during a time corresponding to the summer months when consumers are using additional electricity to combat the higher temperatures.

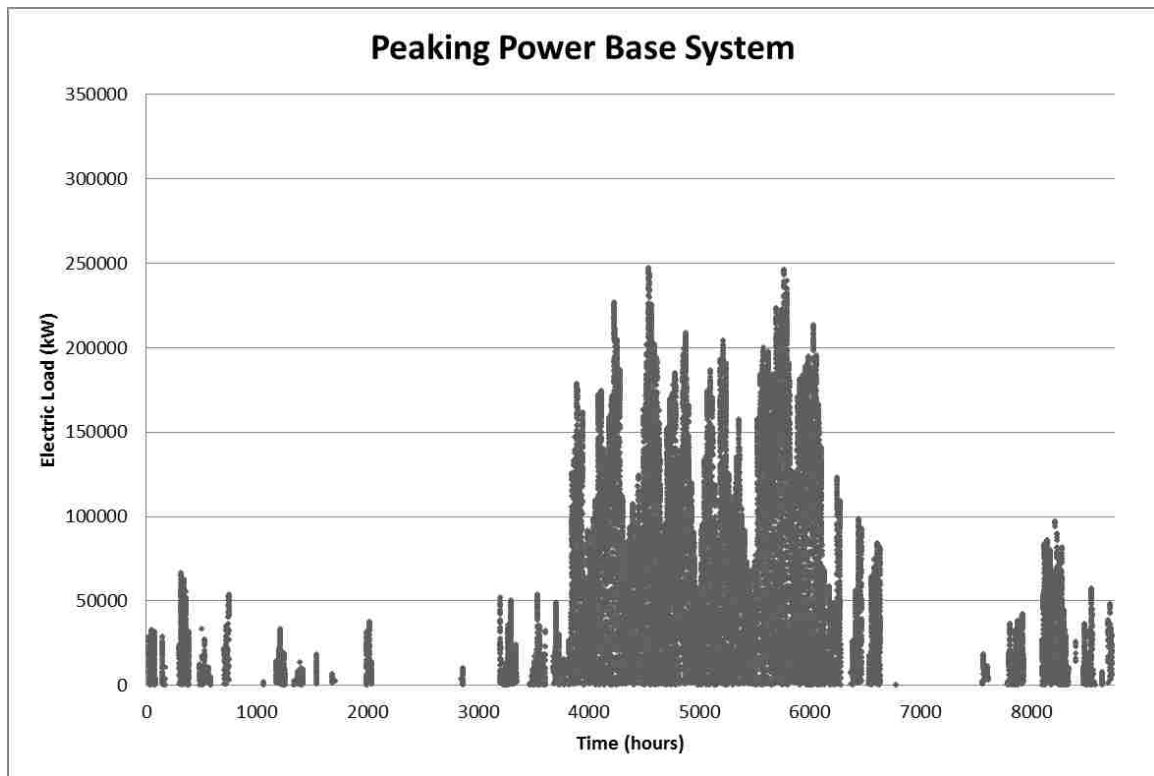


Figure 3.2. Peak Power Demand for Base Hybrid System.

When surplus power is available, the HTSE reduces carbon dioxide emissions and generates syngas. Figure 3.3 and Figure 3.4 show the carbon dioxide emissions and syngas produced, respectively. The figures show that as the day and night cycles and weather patterns change throughout the year that the HTSE operates variably. During the summer months when peak demand is high, the HTSE still operates due to the dynamic

nature of the wind and demand cycle. Figure 3.5 through Figure 3.8 show the comparative differences between each hybrid system. As power production increased the amount of power necessary to match peak demand was reduced. For the hybrid system with an additional PCFB unit, carbon dioxide emissions rose due to the increased combustion of coal. The converse was true for the system with one fewer PCFB unit. Hybrid systems with higher surpluses of electricity reduced carbon dioxide emissions further and produced higher amounts of syngas. For comparison, the hybrid systems were evaluated against another hybrid system that does not utilize an HTSE unit and against a conventional coal based power plant that has the same base load capacity as the compared hybrid system. This type of basis allowed for an economic evaluation that looked at not only the hybrid system, but how the system might perform against conventional technologies and any future possibilities of carbon taxation. The total amounts of carbon dioxide emitted and syngas produced for the various simulated hybrid systems are summarized in Table 3.1. See Appendix A for the remaining hybrid system results.



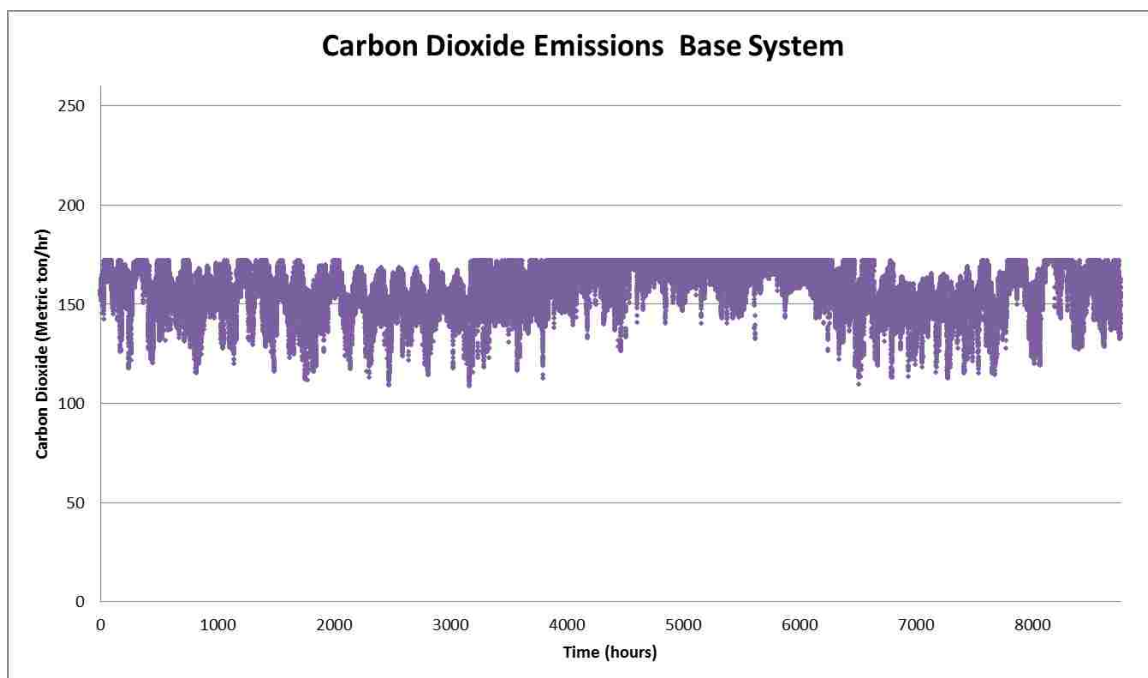


Figure 3.3. Carbon Dioxide Emissions for Base Hybrid System.

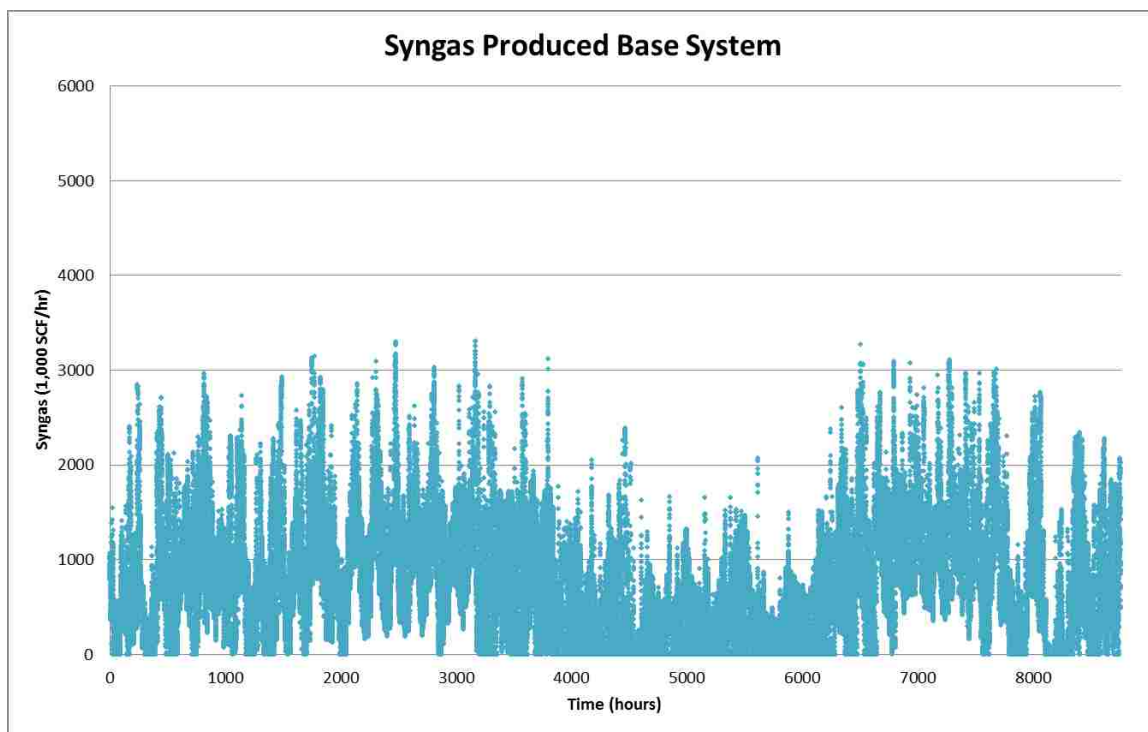


Figure 3.4. Syngas Production of Base Hybrid System.

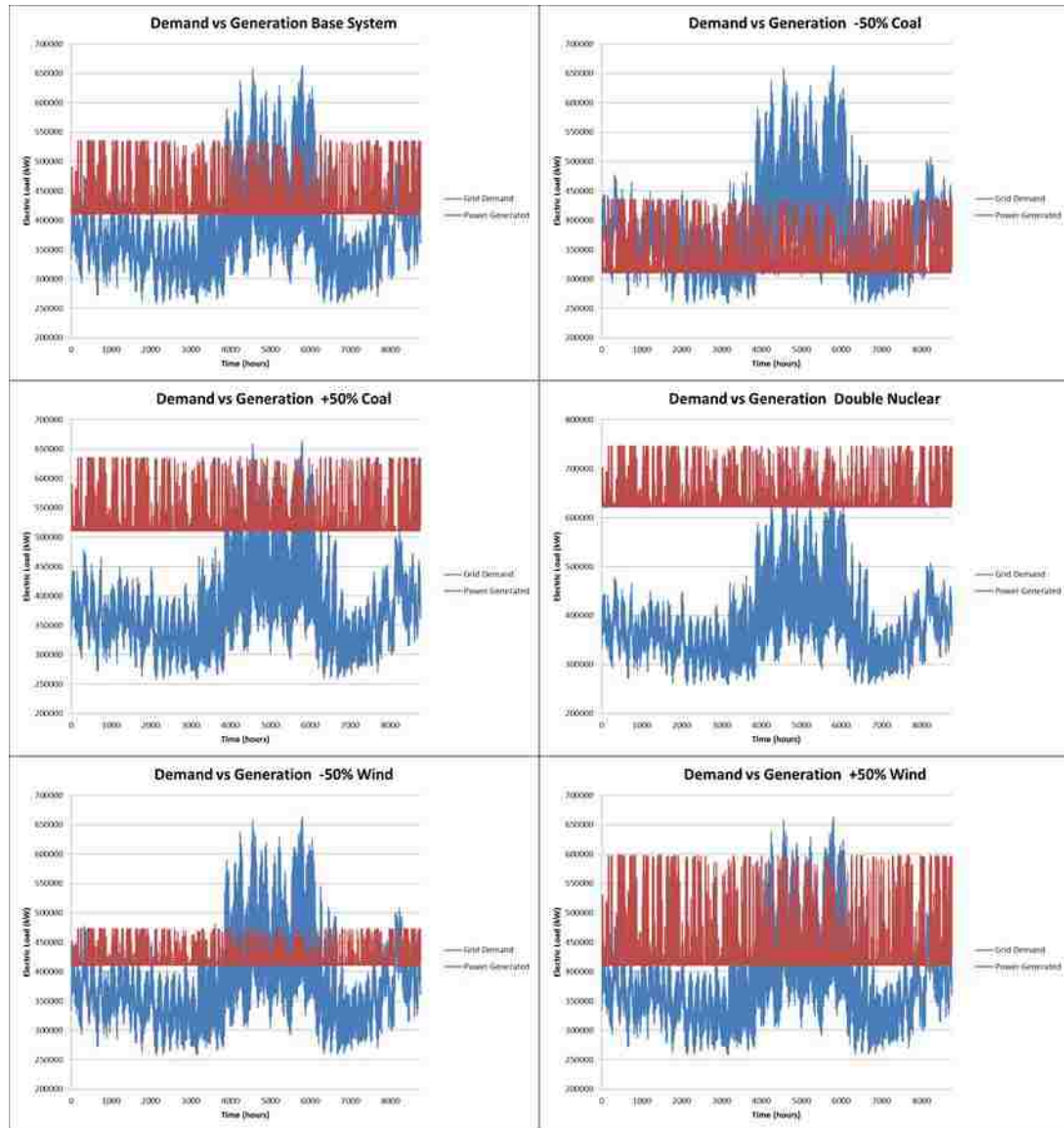


Figure 3.5. Grid Demand versus generation comparison.

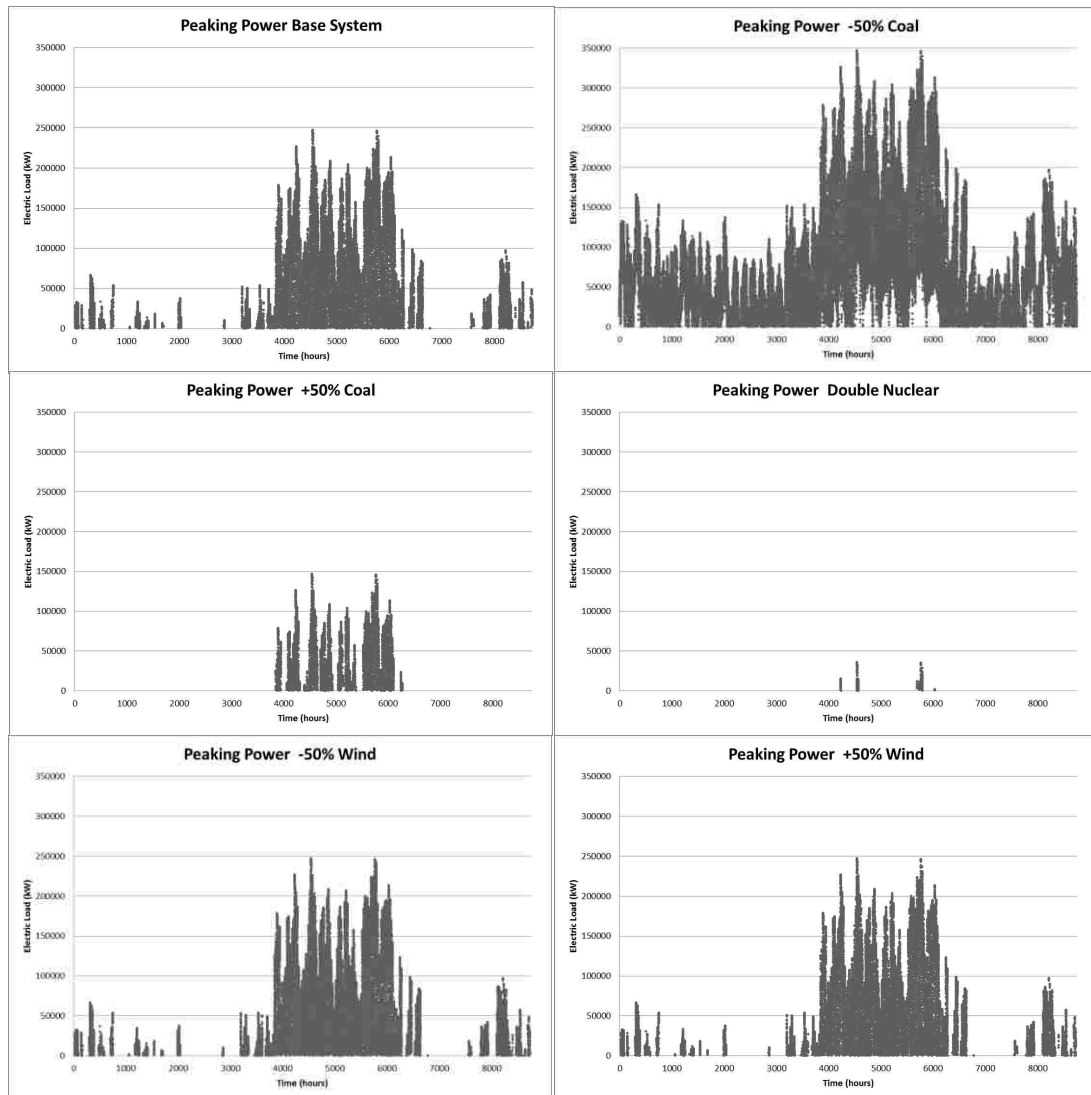


Figure 3.6. Peaking power comparison.

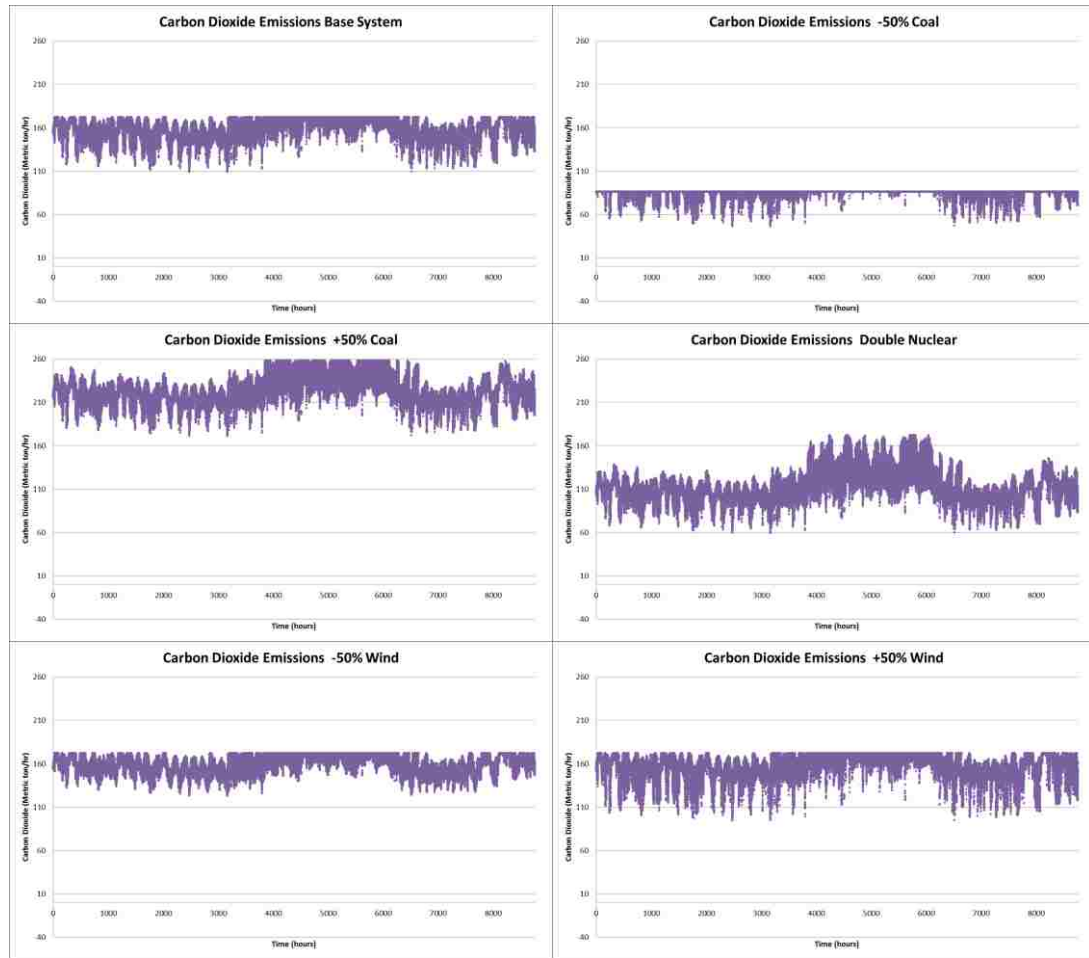


Figure 3.7. Carbon dioxide emissions comparison.

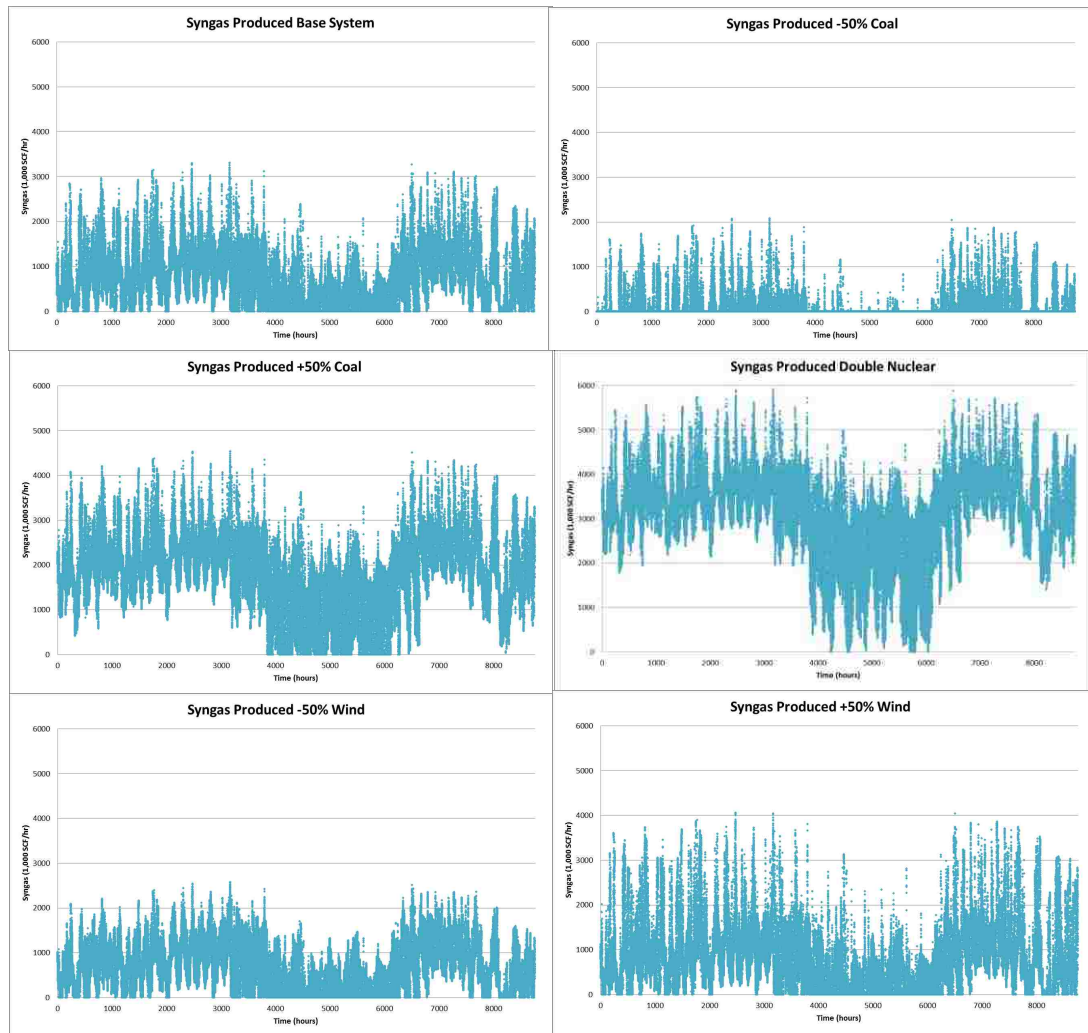


Figure 3.8. Syngas produced comparison.

Table 3.1. Yearly Gases Emitted and Produced.

	Total CO <sub>2</sub> Emitted (metric ton)	Total Syngas Generated (1,000 SCF)
Base System	1,384,395	6,397,876
No HTSE	1,506,577	-
Conventional Coal	3,096,015	-
-50% Coal	735,713	923,058
No HTSE	753,288	-
Conventional Coal	2,342,727	-
+50% Coal	1,959,669	15,711,944
No HTSE	2,259,865	-
Conventional Coal	3,849,304	-
Double Nuclear	983,951	27,341,194
No HTSE	1,506,577	-
Conventional Coal	4,685,454	-
-50% Wind	1,399,754	5,594,565
No HTSE	1,506,577	-
Conventional Coal	3,096,015	-
+50% Wind	1,368,641	7,221,806
No HTSE	1,506,577	-
Conventional Coal	3,096,015	-

#### 4. ECONOMIC EVALUATION

To evaluate the hybrid energy system, this work compares the results to a generic conventional coal base load generator. The conventional coal system is also paired with a wind power generator in order to keep peak demand the same. This approach evaluates the hybridization of the PCFB and SMR systems with the HTSE. Having the conventional coal system with a wind generator allows the hybrid system comparison to show its chemical storage ability.

The Energy Information Administration (EIA) summarizes different generating technologies for comparison in the Annual Energy Outlook. In this report, the levelized cost of electricity (LCOE) is used to compare per-kilowatt hour costs of different generating sources broken down into several factors [18]. Table 4.1 summarizes the factors and LCOE used in this work. In the Annual Energy Outlook, the EIA places a 3% increase in capital costs to represent a \$15 per metric ton of carbon dioxide tax. This work analyzes a potential carbon tax separately and has removed that increase. This work also follows the EIA model and uses a weighted average cost of capital rate of 6.1% for present value calculations.

The High Temperature Steam Co-Electrolysis unit reacts carbon dioxide with steam to generate syngas. Solid Oxide Fuel Cells (SOFC) take a fuel such as natural gas and generates electricity and combustion products. Since these technologies are similarly related, a cost study performed by the Pacific Northwest National Laboratory is used to evaluate the HTSE [19]. This cost study assumes economies of scale are achieved through the mass production of SOFC units after the technology has reached certain performance targets [20].

Table 4.1. Levelized Cost of Electricity.

Plant Type	Capacity Factor (%)	Levelized Capital Cost	Fixed O&M	Variable O&M	Transmission Investment	Total System LCOE (\$/MWh)
Conventional Coal*	85.0	58.6	4.2	29.4	1.2	93.4
PCFB (Advanced Coal)*	85.0	74.7	6.9	30.7	1.2	113.5
Advanced Nuclear	90.0	70.1	11.8	12.2	1.1	95.2
Wind	36.0	57.7	12.8	0.0	3.1	73.6
Advanced Combustion Turbine*	30.0	27.0	2.7	79.6	3.5	112.8
Solid Oxide Fuel Cell <sup>+</sup>	-	31.9	8.6	0.0	0.0	40.5
* Removed a 3% increase on Capital Costs for carbon emitters based on \$15/metric ton						
+ Used SOFC as base for HTSE from PNNL source [19] converted to 2013 \$						

The idea of a hybrid energy system is different from that of conventional generation plants in that the systems are coupled. Hybrid systems may benefit from certain cost reductions as a result of being combined. In the standard EIA economic model, a generating facility has costs tied to capital, fixed operations and maintenance (O&M), and variable O&M. For the economic analysis presented in this work, potential capital cost reductions of 10%, 20%, and 30% are evaluated. These reductions are based on the idea that the hybrid system may share costs between generation sources such as land, utilities, and manpower.

Another component of the economic evaluation comes in the form of a theoretical carbon dioxide emissions tax. Since the EIA already assumed a \$15 per metric ton of



carbon dioxide tax, this work investigates the cost comparison of no tax to a \$15 and a \$30 per metric ton of carbon dioxide tax. The cost of the tax is applied to the amount of carbon dioxide generated by the model and is then assumed to be the same for each of the 30 years of the systems life span which is the system life assumed by the EIA [8]. This cost is then discounted back to get a net present value of the cost of the tax before it is added to the levelized costs of the systems. An advanced combustion turbine is valued to cover costs associated with peak power demand. The LCOE of each generation source is multiplied by its power produced to get a levelized cost for each system (Table 4.2 - Table 4.3).

Table 4.2. Base Hybrid System Levelized Cost Comparisons (A).

Base System Levelized Cost Comparisons					
Cost Source	Conventional Coal Reference System Levelized Cost (\$)	Hybrid Energy System Levelized Cost No HTSE (\$)	Base Hybrid System Levelized Cost (\$)	10% Hybridization No HTSE (\$)	10% Hybridization (\$)
Conventional Coal	\$336,420,434.80	-	-	-	-
PCFB (Advanced Coal)	-	\$198,782,260.19	\$198,782,260.19	\$67,977,600.00	\$67,977,600.00
Advanced Nuclear	-	\$175,963,872.00	\$175,963,872.00	\$46,393,836.00	\$46,393,836.00
Wind	\$10,871,071.88	\$10,871,071.88	\$10,871,071.88	\$10,871,071.88	\$10,871,071.88
Advanced Combustion Turbine	\$16,788,788.30	\$16,788,788.30	\$16,788,788.30	\$16,788,788.30	\$16,788,788.30
Solid Oxide Fuel Cell	-	-	\$21,030,156.92	-	\$21,030,156.92
Hybridized Capital Cost	-	-	-	\$234,337,226.57	\$234,337,226.57
\$15/Metric ton CO2	\$678,899,944.50	\$330,364,936.49	\$303,572,599.47	\$330,364,936.49	\$303,572,599.47
\$30/Metric ton CO2	\$1,357,799,888.99	\$660,729,872.99	\$607,145,198.94	\$660,729,872.99	\$607,145,198.94
Total Cost	\$364,080,294.98	\$402,405,992.38	\$423,436,149.30	\$376,368,522.76	\$397,398,679.68
Total Cost + \$15 tax	\$1,042,980,239.48	\$732,770,928.87	\$727,008,748.77	\$706,733,459.25	\$700,971,279.15
Total Cost + \$30 tax	\$1,721,880,183.97	\$1,063,135,865.37	\$1,030,581,348.24	\$1,037,098,395.75	\$1,004,543,878.62

Table 4.3. Base Hybrid System Levelized Cost Comparisons (B).

Base System Levelized Cost Comparisons				
Cost Source	20% Hybridization No HTSE (\$)	20% Hybridization (\$)	30% Hybridization No HTSE (\$)	30% Hybridization (\$)
Conventional Coal	-	-	-	-
PCFB (Advanced Coal)	\$67,977,600.00	\$67,977,600.00	\$67,977,600.00	\$67,977,600.00
Advanced Nuclear	\$46,393,836.00	\$46,393,836.00	\$46,393,836.00	\$46,393,836.00
Wind	\$10,871,071.88	\$10,871,071.88	\$10,871,071.88	\$10,871,071.88
Advanced Combustion Turbine	\$16,788,788.30	\$16,788,788.30	\$16,788,788.30	\$16,788,788.30
Solid Oxide Fuel Cell	-	\$21,030,156.92	-	\$21,030,156.92
Hybridized Capital Cost	\$208,299,756.96	\$208,299,756.96	\$182,262,287.34	\$182,262,287.34
\$15/Metric ton CO2	\$330,364,936.49	\$303,572,599.47	\$330,364,936.49	\$303,572,599.47
\$30/Metric ton CO2	\$660,729,872.99	\$607,145,198.94	\$660,729,872.99	\$607,145,198.94
Total Cost	\$350,331,053.14	\$371,361,210.06	\$324,293,583.52	\$345,323,740.44
Total Cost + \$15 tax	\$680,695,989.63	\$674,933,809.53	\$654,658,520.01	\$648,896,339.91
Total Cost + \$30 tax	\$1,011,060,926.13	\$978,506,409.00	\$985,023,456.51	\$952,468,939.38

The value of the syngas produced by the hybrid systems which utilize the HTSE can be evaluated by comparing the hybrid system to the conventional coal system. The levelized cost of the hybrid system is subtracted from the cost of the conventional coal system. This difference is the value the syngas must achieve in order to reduce the cost of the hybrid system to that of the conventional coal system (Table 4.4). This syngas value is then amortized over the life of the system to calculate the sale price per unit of syngas to match the conventional coal system costs (Table 4.5). See Appendix B for the remaining hybrid system evaluations.

Table 4.4. Value of Syngas for Base Hybrid System.

	Value of Syngas Produced to Match Conventional Coal Cost for Base System			
	Base Hybrid System (\$)	10% Hybridization (\$)	20% Hybridization (\$)	30% Hybridization (\$)
No Tax	\$59,355,854	\$33,318,384	\$7,280,915	-\$18,756,554
\$15/Metric ton CO <sub>2</sub>	-\$315,971,490	-\$342,008,960	-\$368,046,429	-\$394,083,899
\$30/Metric ton CO <sub>2</sub>	-\$691,298,835	-\$717,336,305	-\$743,373,774	-\$769,411,244

Table 4.5. Syngas Sale Price for Base Hybrid System.

	Syngas Sale Price to Match Conventional Coal Cost for Base System			
	Base Hybrid System (\$/1000 SCF)	10% Hybridization (\$/1000 SCF)	20% Hybridization (\$/1000 SCF)	30% Hybridization (\$/1000 SCF)
No Tax	\$0.63	\$0.36	\$0.08	Profitable at any
\$15/Metric ton CO <sub>2</sub>	Profitable at any	Profitable at any	Profitable at any	Profitable at any
\$30/Metric ton CO <sub>2</sub>	Profitable at any	Profitable at any	Profitable at any	Profitable at any

## 5. CONCLUSIONS

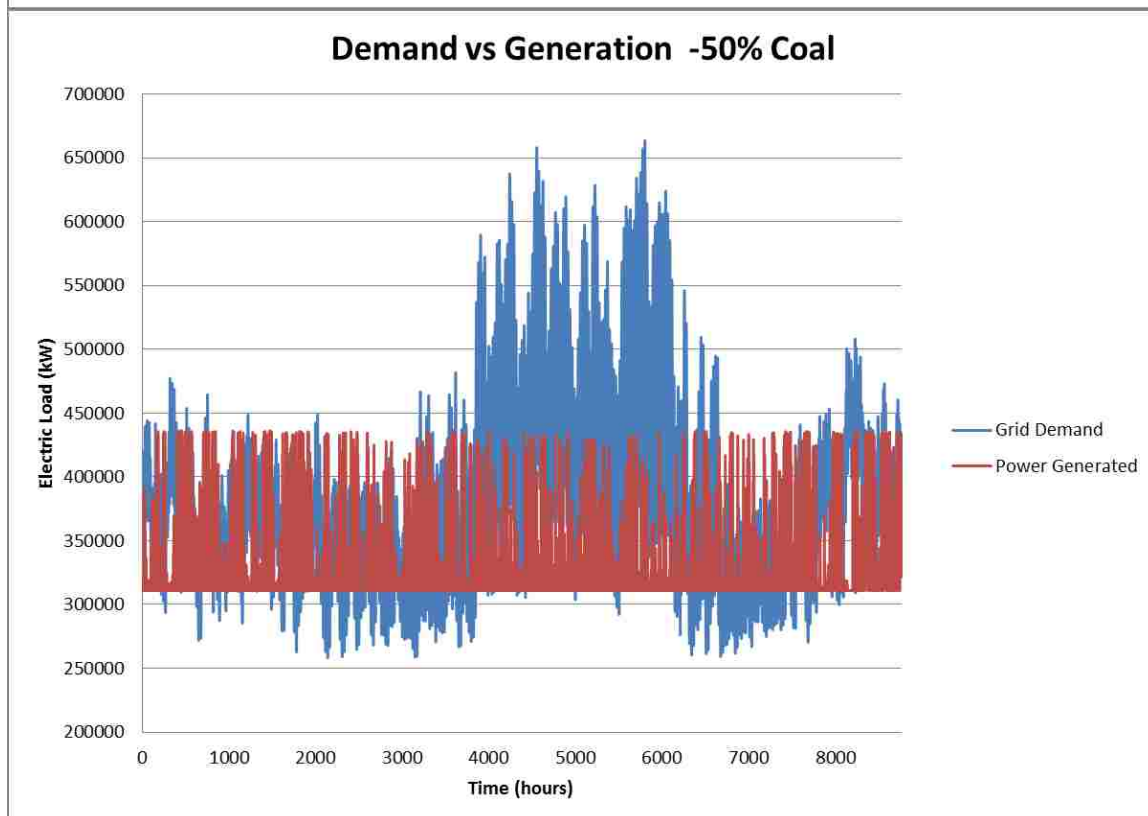
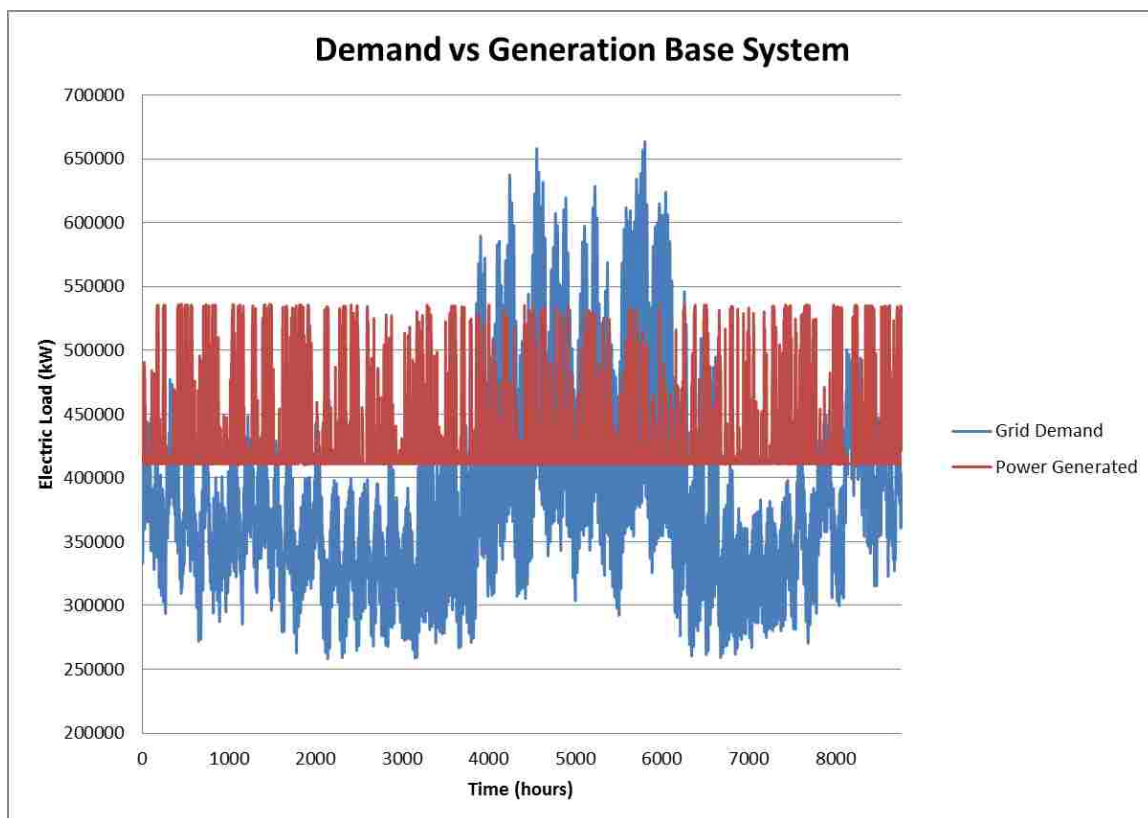
Based on the simulation results, the proposed hybrid energy system is capable of producing syngas all year, including during high peak demand, by capturing excess energy during the day and night cycle and during high wind power generation. Keeping in mind that the SOFC and SMR markets [21] need to reach technology targets and economies of scale, the hybrid system utilizing next generation technologies can be economically competitive with conventional power generation sources. The hybrid system cost reductions have a large impact on the potential costs of the systems. The value of the syngas produced can make a hybrid system viable versus conventional coal technologies. When compared against conventional coal technology, the hybrid system remains competitive with a syngas sale price between \$0.33 and \$1.77 per 1,000 SCF dependent upon the hybrid system configuration. The inclusion of a carbon dioxide emissions tax immediately makes the hybrid system an economical alternative to conventional coal generation due to the reduced carbon emissions from utilizing SMR nuclear technology alongside mitigating carbon emissions with the HTSE.

## 6. FUTURE WORK

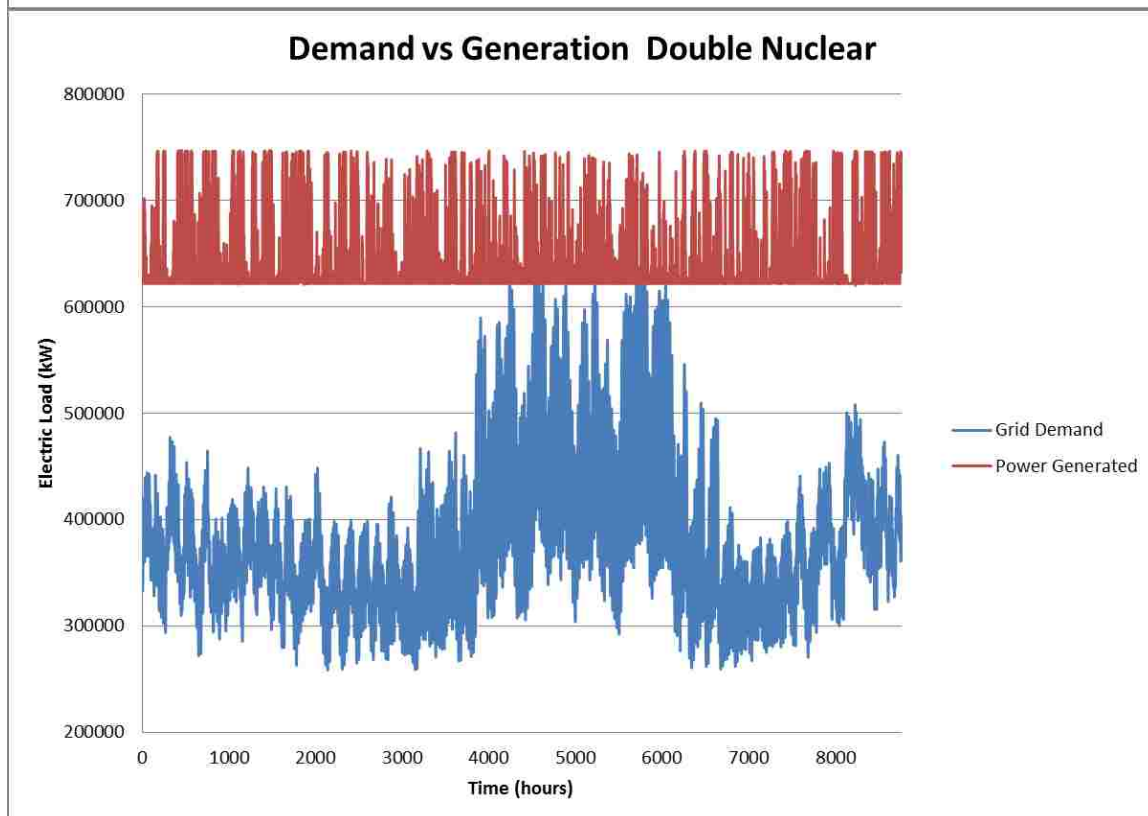
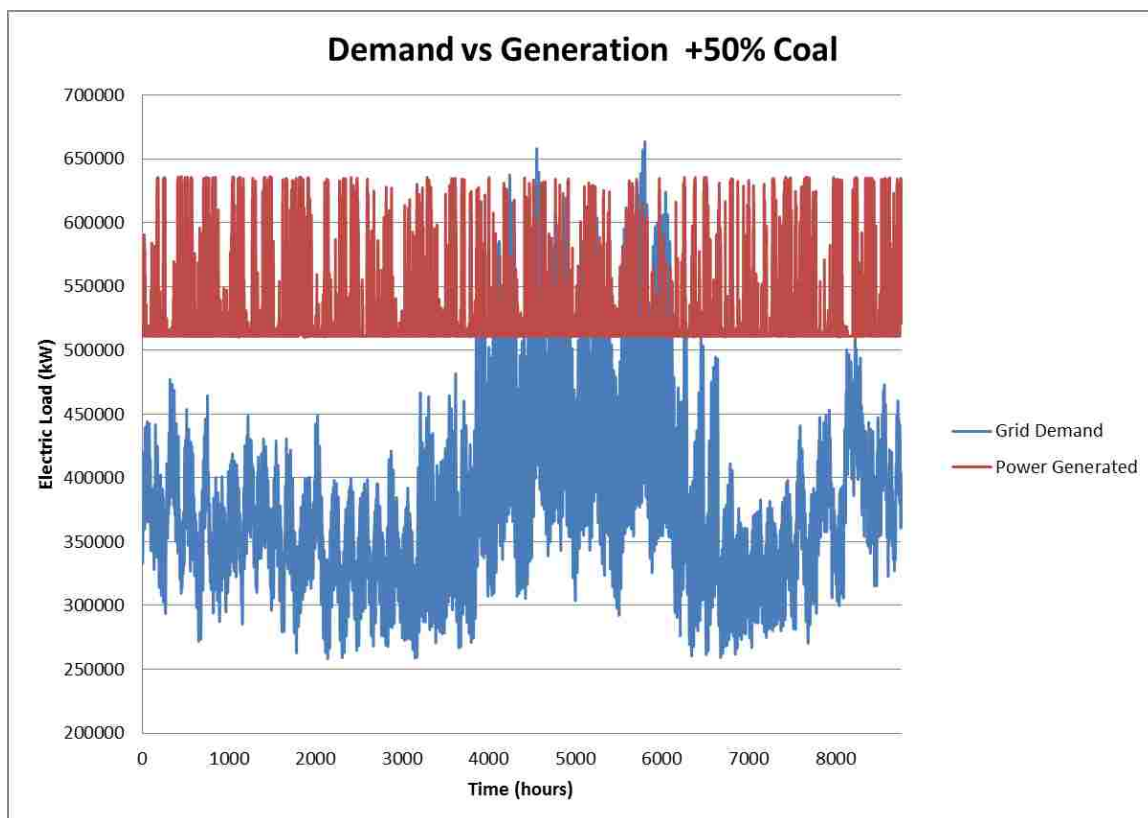
The current work only analyzes six different potential hybrid systems on a fixed range of grid demand. Future work could expand upon this and optimize the hybrid system by varying units in the system together rather than one at a time such as more or less coal coupled with more or less nuclear and wind. The PCFB is capable of utilizing biomass as a feedstock, with modified fuel costs and emissions. This work compares a hybrid system with a conventional coal system which produces a lot of carbon dioxide. Future work could compare the hybrid system to a nuclear base load generator that would face no carbon dioxide emissions penalty. A hypothetical carbon dioxide tax could potentially make the carbon based part of the hybrid system too costly. A hybrid system consisting of nuclear and renewables with an HTSE system that only generates hydrogen could be considered. This work stops production at syngas, yet future work could use this as a feedstock to generate more valuable products such as synfuels. An in depth analysis of a hypothetical hybrid facility could be performed to see how much cost reduction could actually be achieved. The current dynamic model could be modified to handle solar PV cells instead of wind turbines to generate renewable electricity.

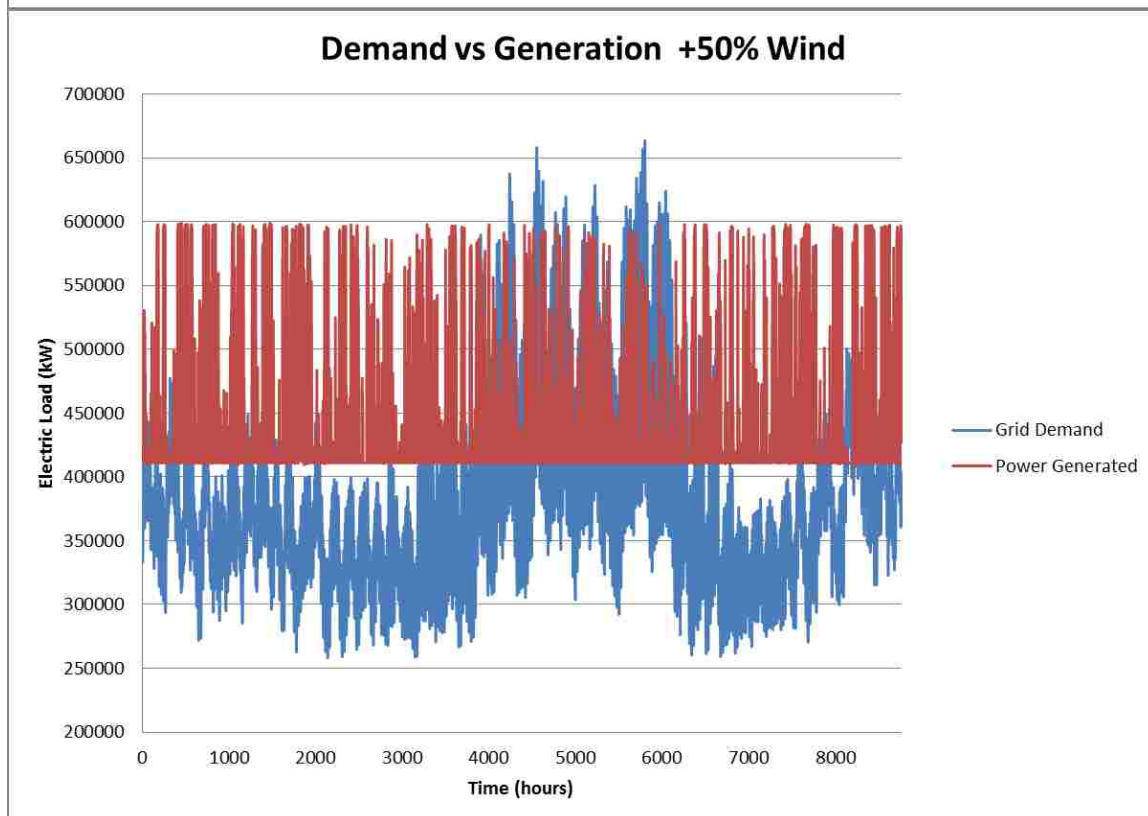
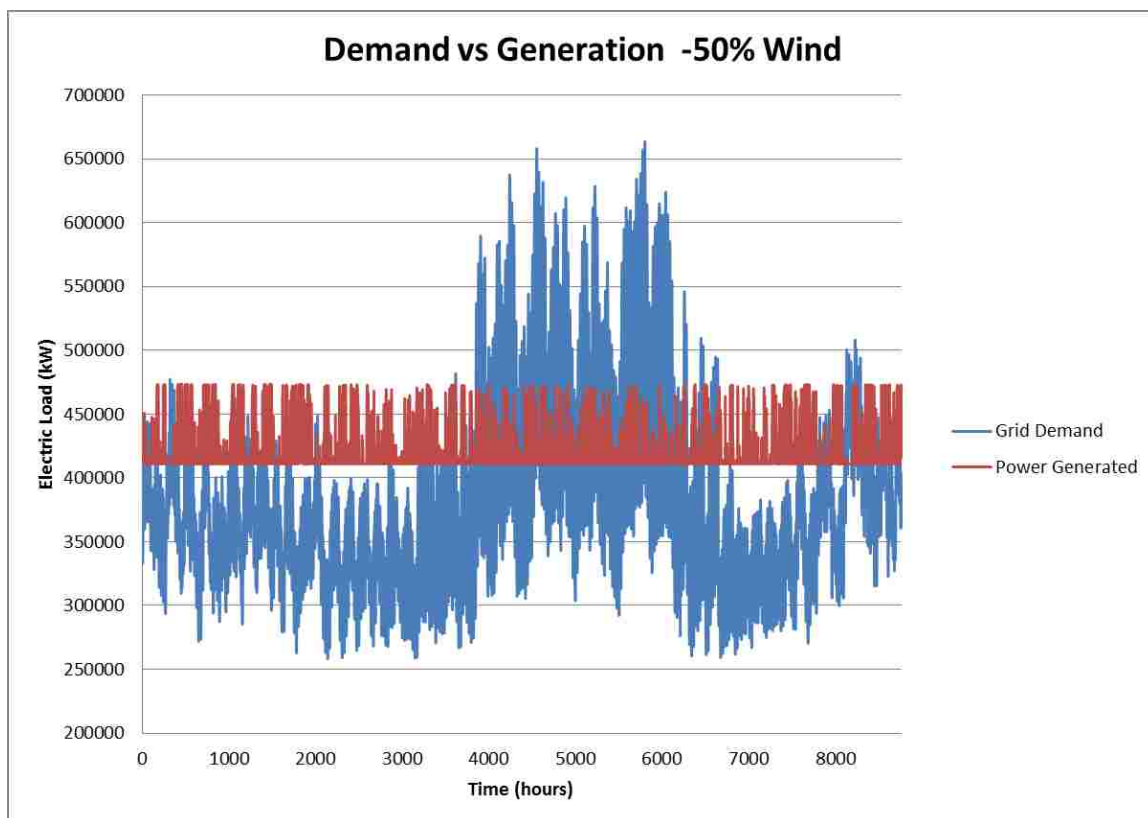
**APPENDIX A.**

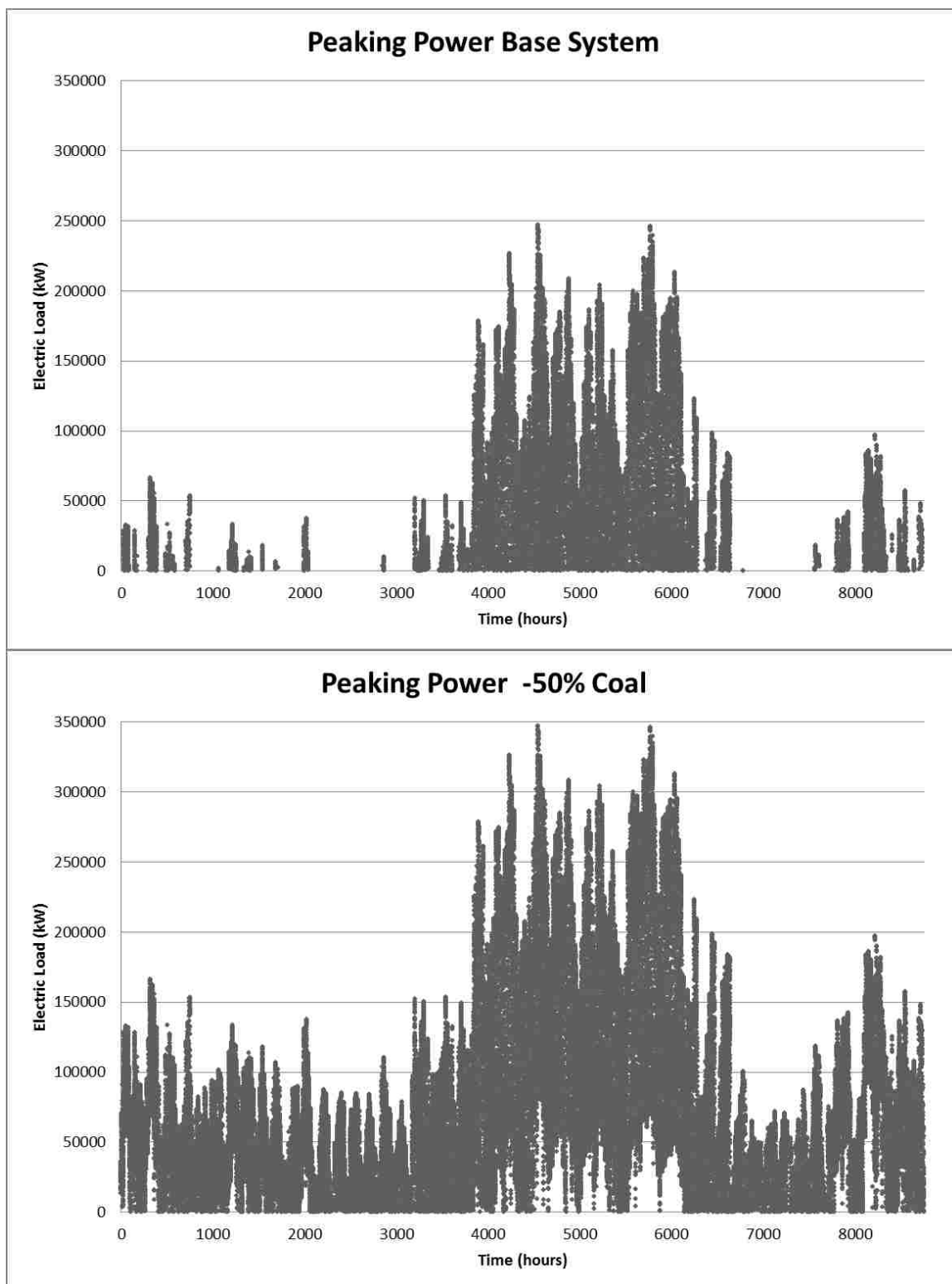
**HYBRID ENERGY SYSTEM DYNAMIC SIMULATION RESULTS**

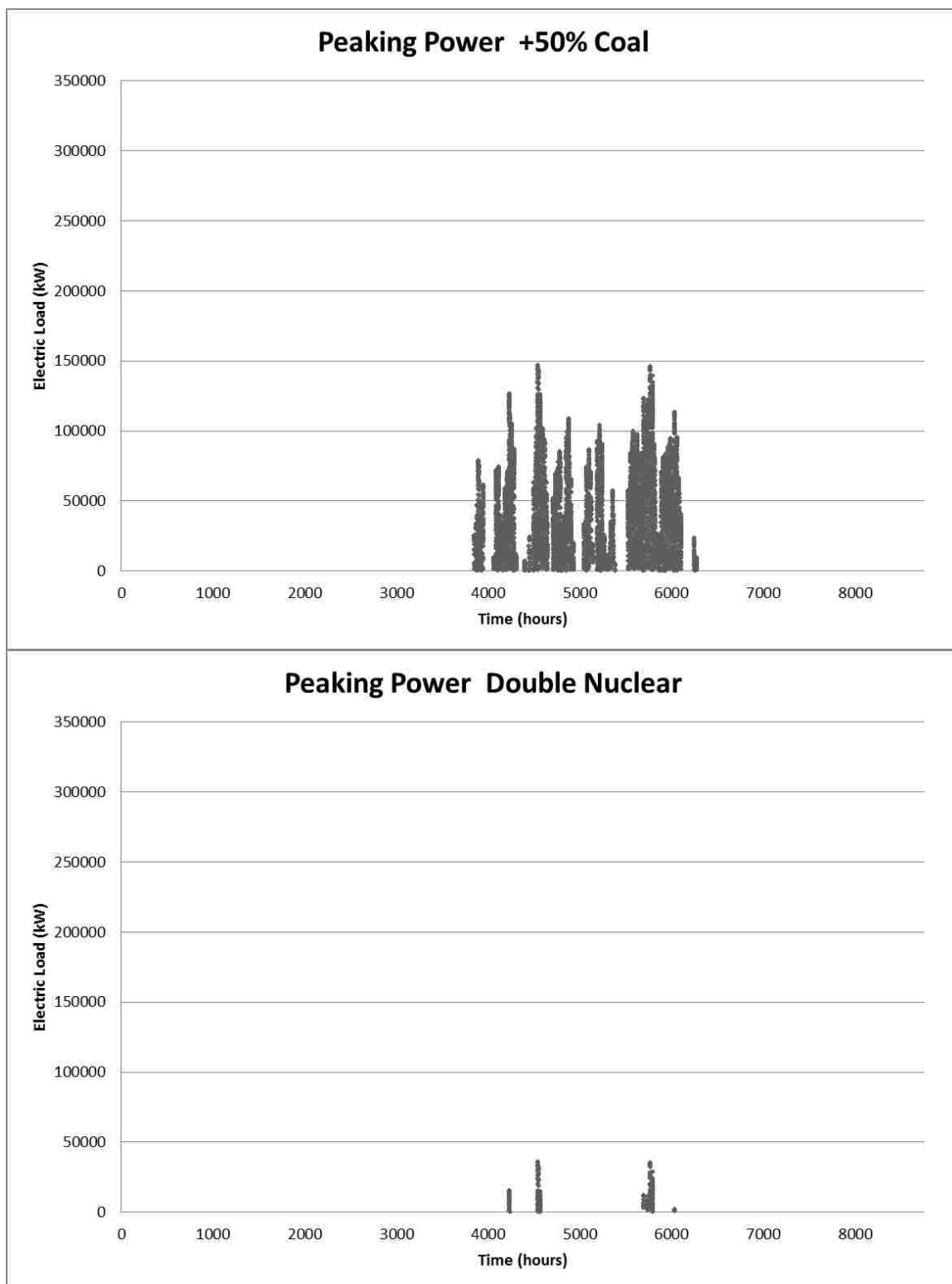


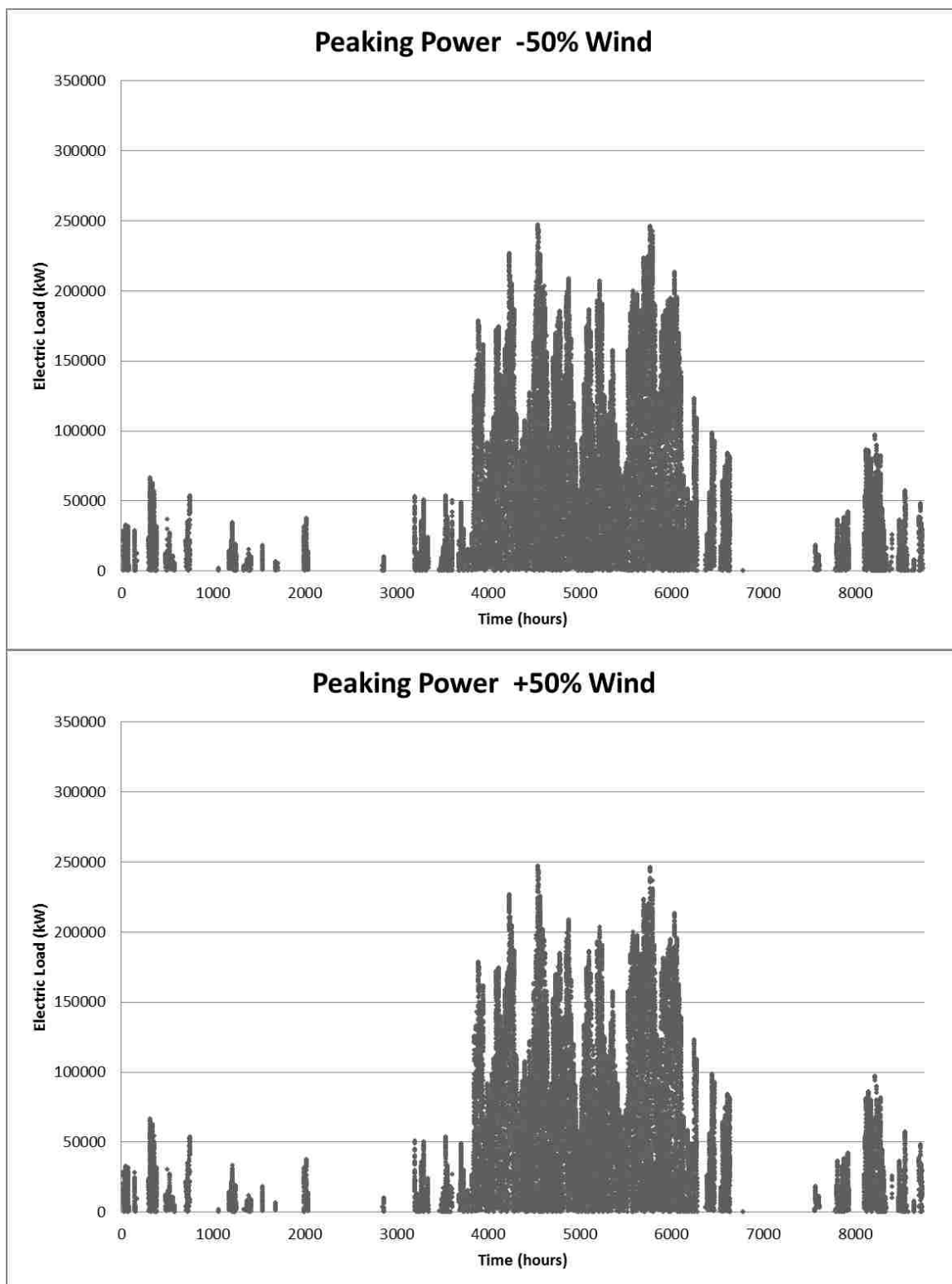


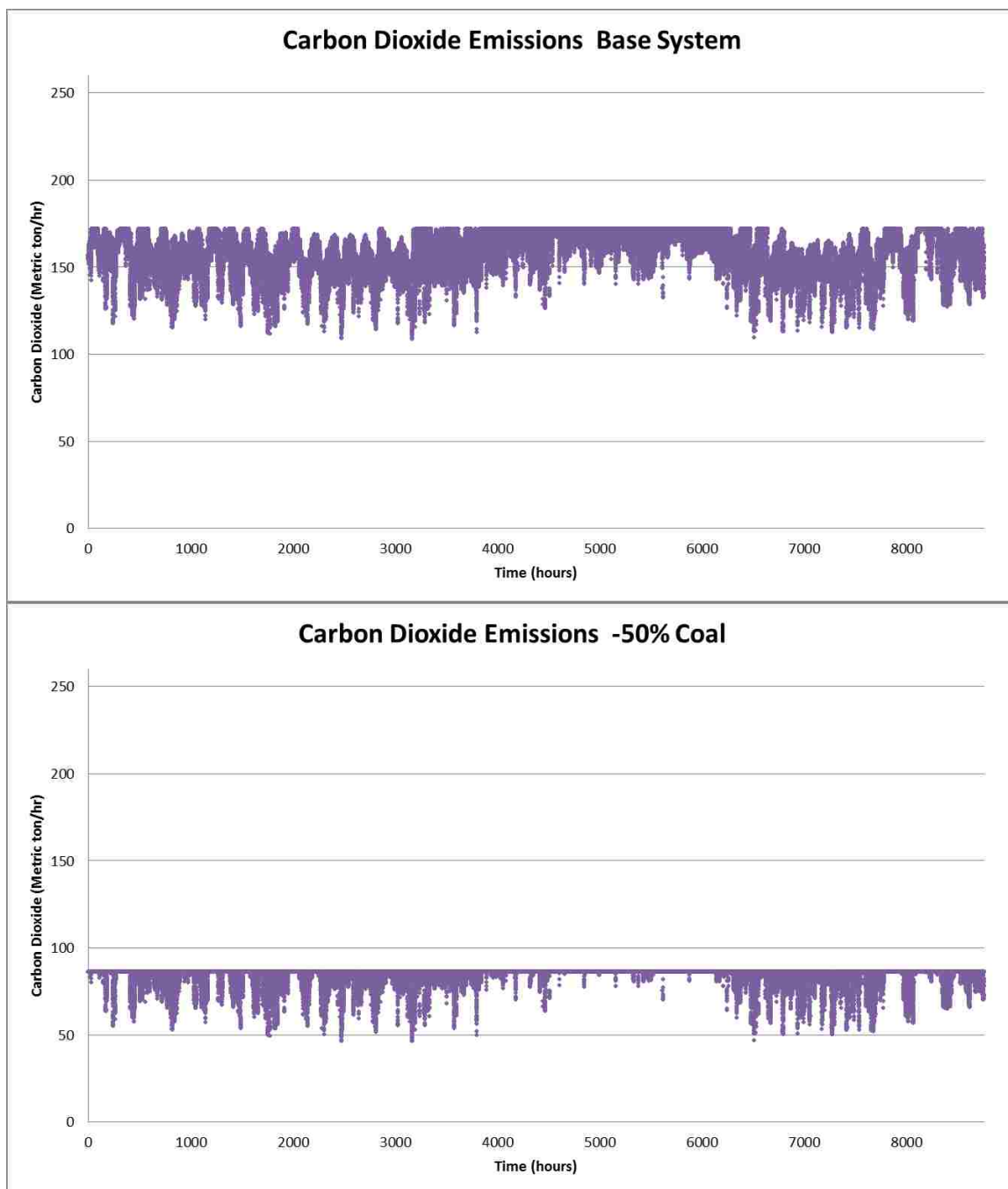


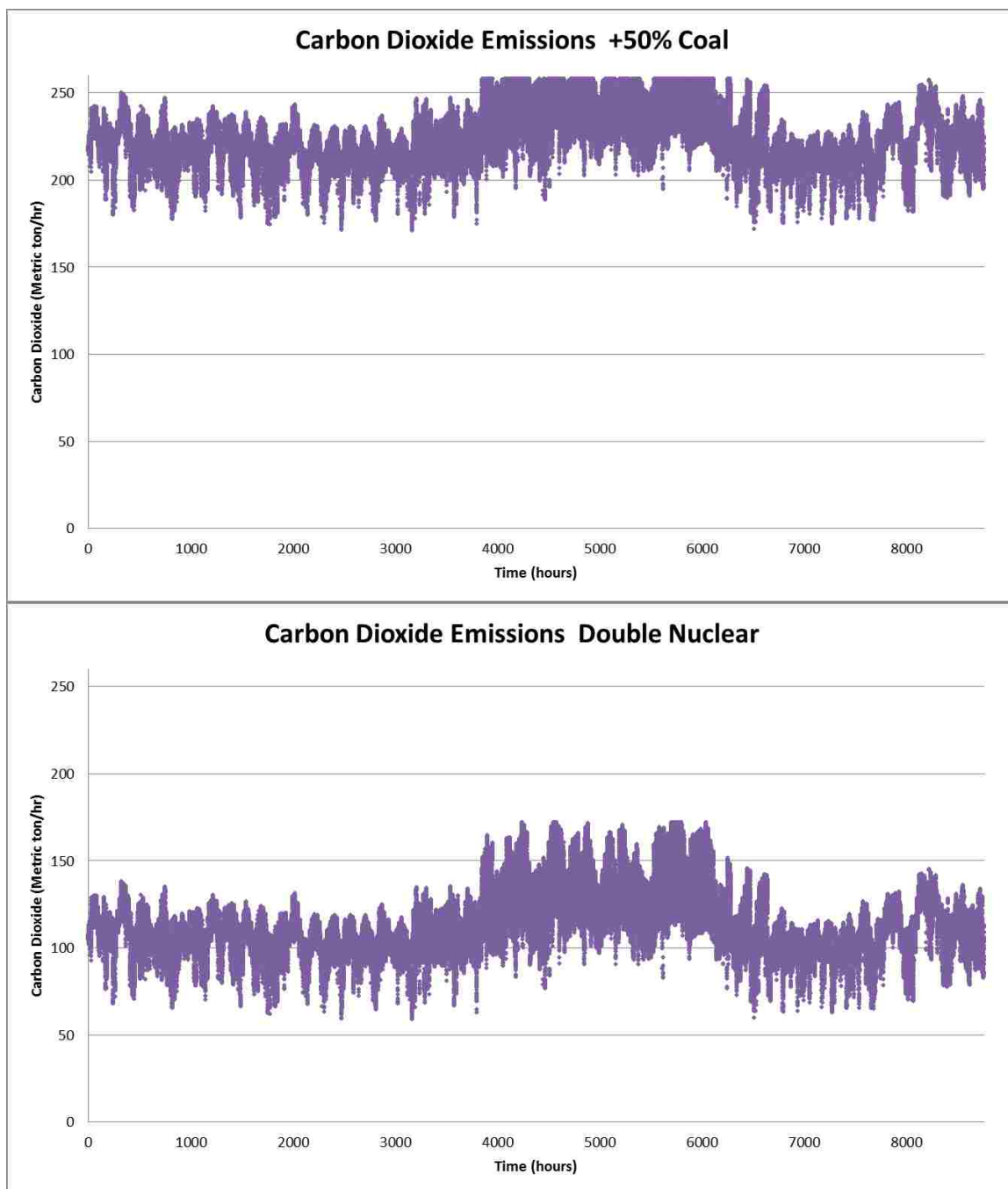


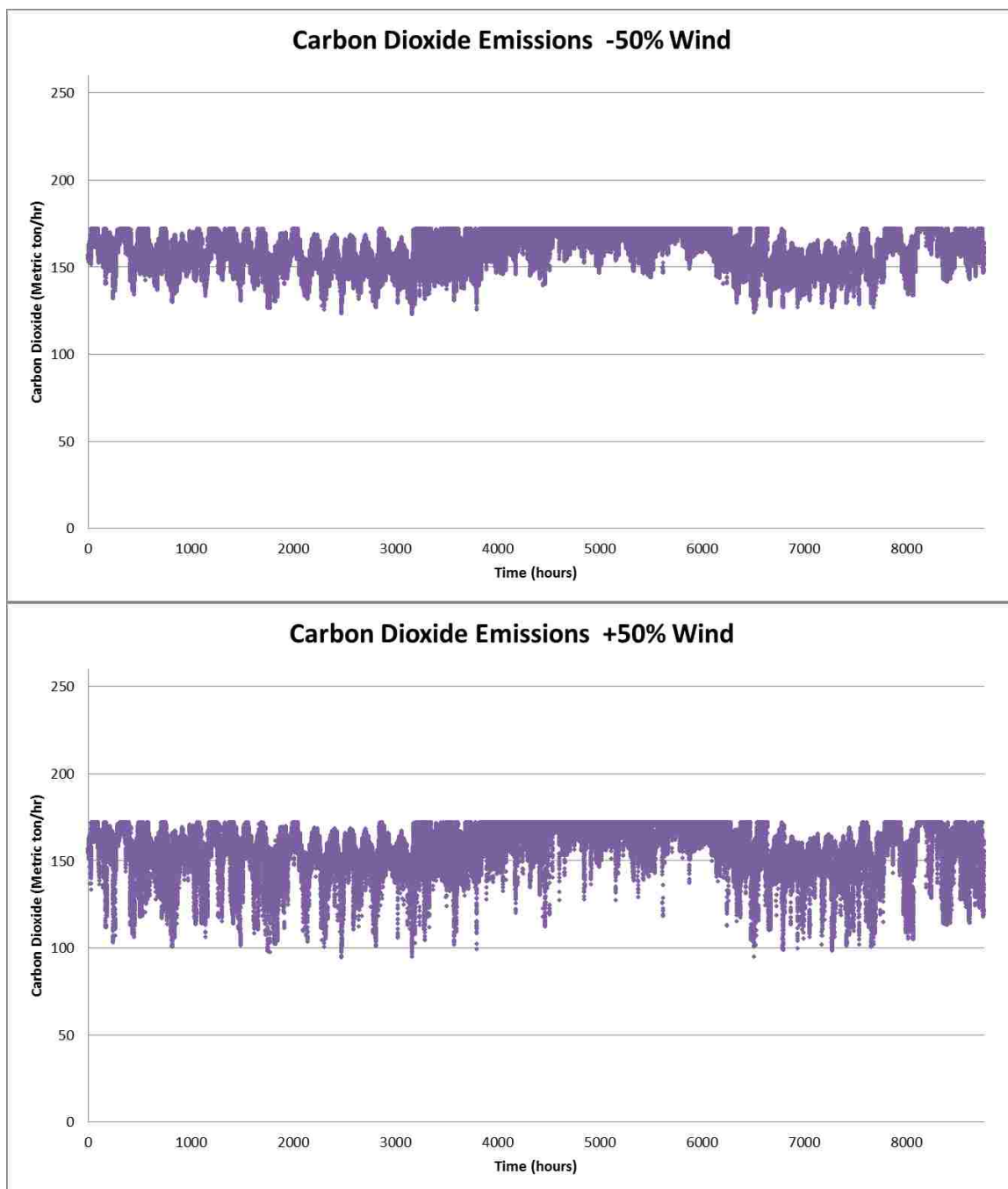




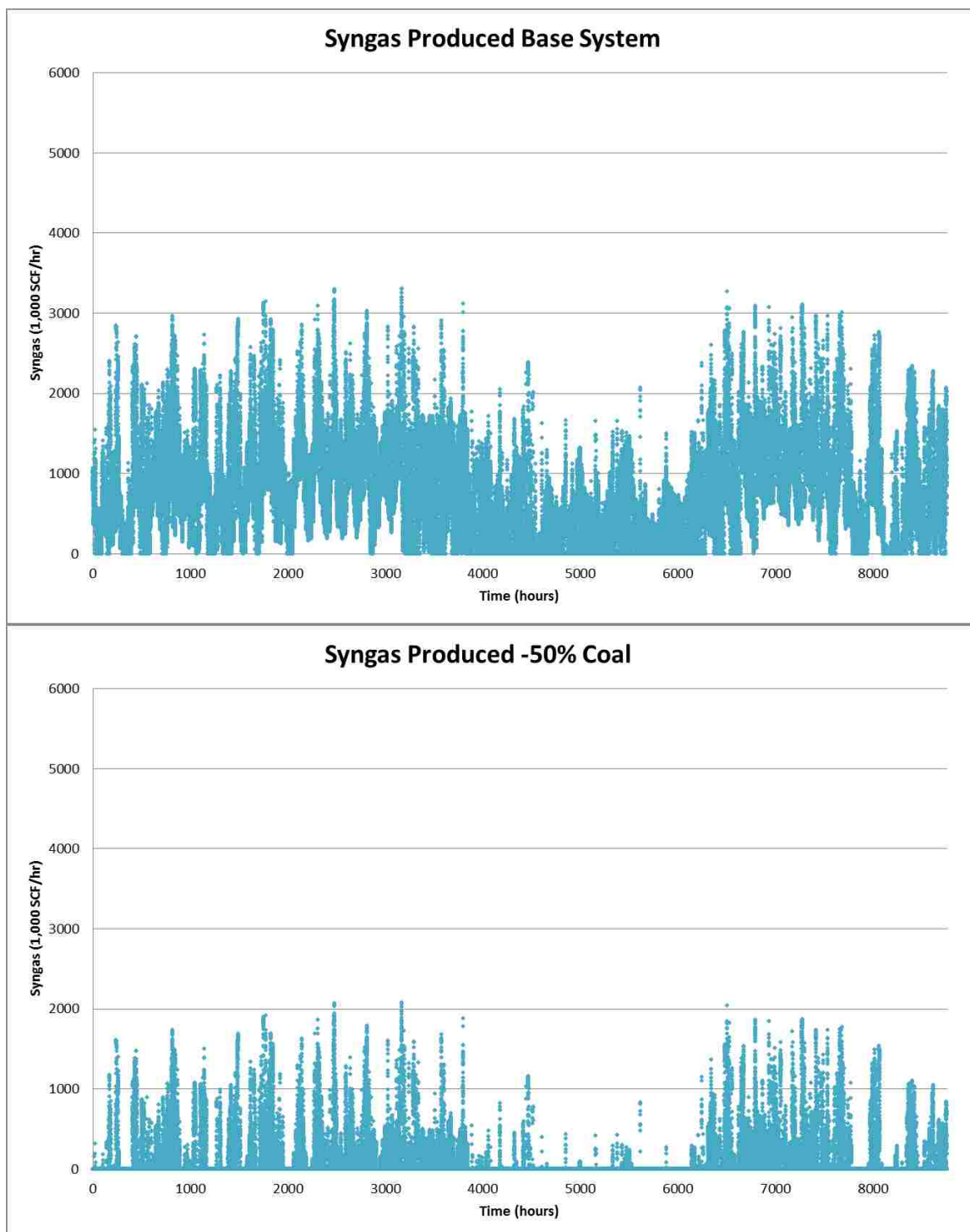


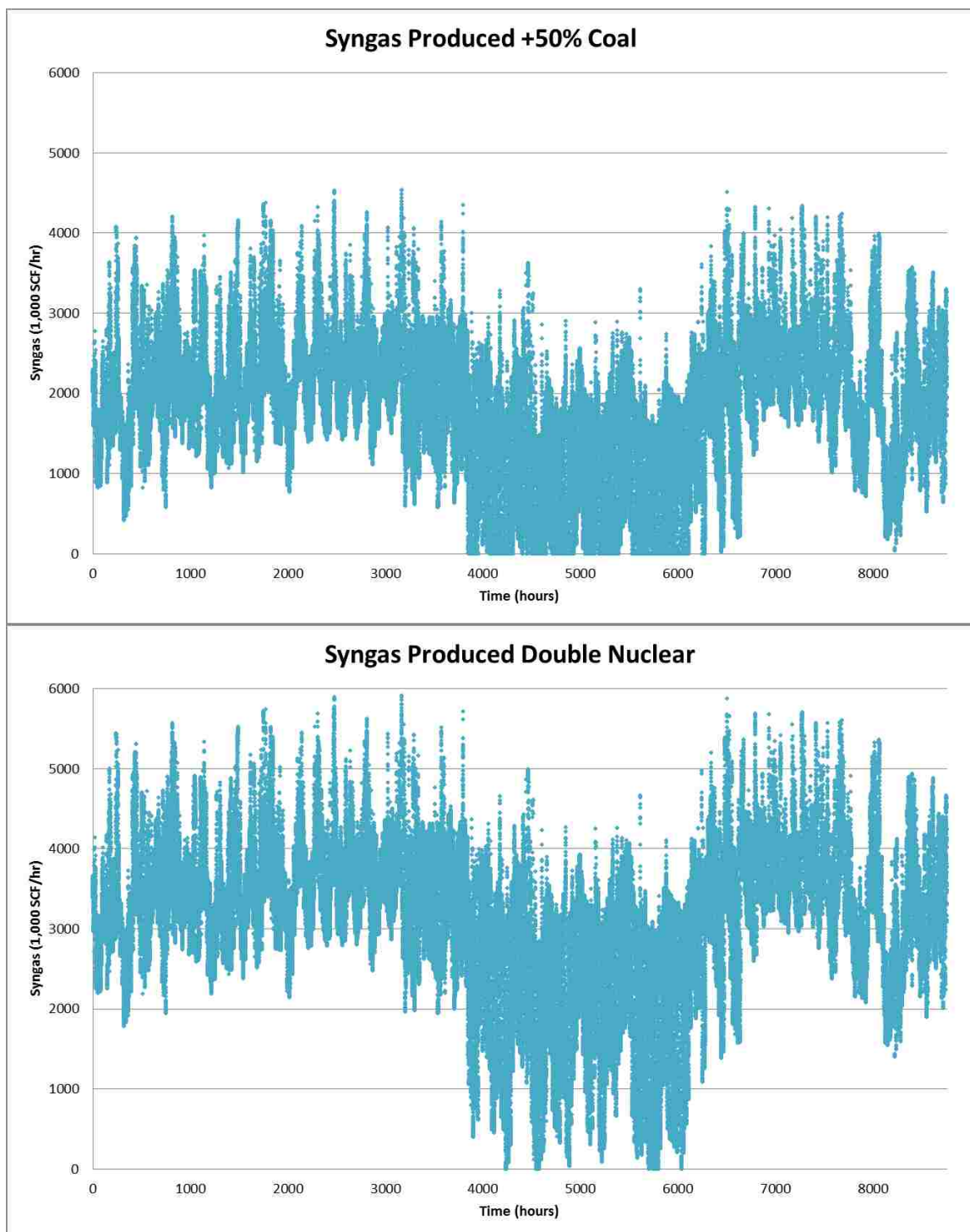


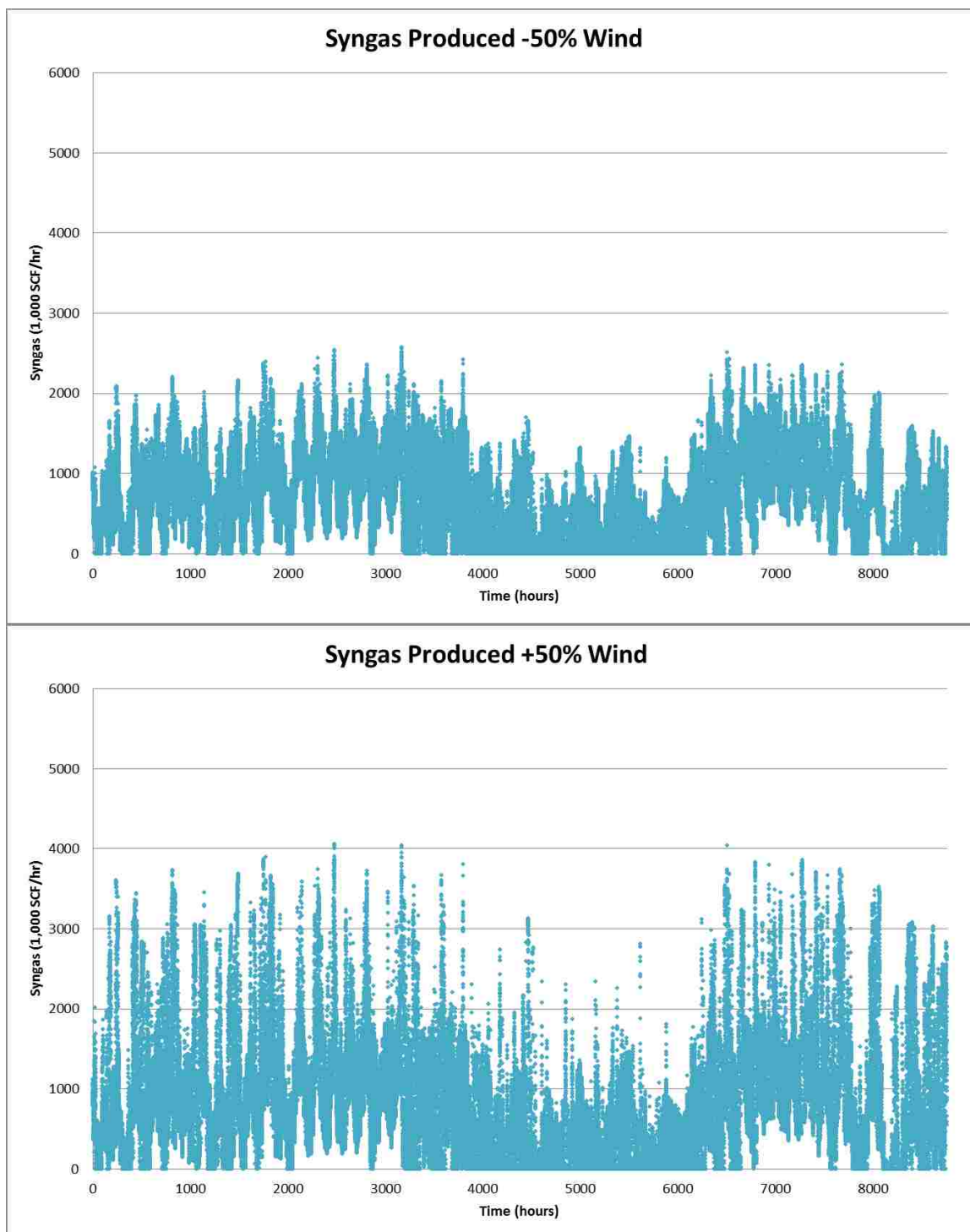












**APPENDIX B.**  
**HYBRID ENERGY SYSTEM ECONOMIC EVALUATIONS**

Base System Levelized Cost Comparisons					
Cost Source	Conventional Coal Reference System Levelized Cost (\$)	Hybrid Energy System Levelized Cost No HTSE (\$)	Base Hybrid System Levelized Cost (\$)	10% Hybridization No HTSE (\$)	10% Hybridization (\$)
Conventional Coal	\$336,420,434.80	-	-	-	-
PCFB (Advanced Coal)	-	\$198,782,260.19	\$198,782,260.19	\$67,977,600.00	\$67,977,600.00
Advanced Nuclear	-	\$175,963,872.00	\$175,963,872.00	\$46,393,836.00	\$46,393,836.00
Wind	\$10,871,071.88	\$10,871,071.88	\$10,871,071.88	\$10,871,071.88	\$10,871,071.88
Advanced Combustion Turbine	\$16,788,788.30	\$16,788,788.30	\$16,788,788.30	\$16,788,788.30	\$16,788,788.30
Solid Oxide Fuel Cell	-	-	\$21,030,156.92	-	\$21,030,156.92
Hybridized Capital Cost	-	-	-	\$234,337,226.57	\$234,337,226.57
\$15/Metric ton CO2	\$678,899,944.50	\$330,364,936.49	\$303,572,599.47	\$330,364,936.49	\$303,572,599.47
\$30/Metric ton CO2	\$1,357,799,888.99	\$660,729,872.99	\$607,145,198.94	\$660,729,872.99	\$607,145,198.94
Total Cost	\$364,080,294.98	\$402,405,992.38	\$423,436,149.30	\$376,368,522.76	\$397,398,679.68
Total Cost + \$15 tax	\$1,042,980,239.48	\$732,770,928.87	\$727,008,748.77	\$706,733,459.25	\$700,971,279.15
Total Cost + \$30 tax	\$1,721,880,183.97	\$1,063,135,865.37	\$1,030,581,348.24	\$1,037,098,395.75	\$1,004,543,878.62

Base System Levelized Cost Comparisons				
Cost Source	20% Hybridization No HTSE (\$)	20% Hybridization (\$)	30% Hybridization No HTSE (\$)	30% Hybridization (\$)
Conventional Coal	-	-	-	-
PCFB (Advanced Coal)	\$67,977,600.00	\$67,977,600.00	\$67,977,600.00	\$67,977,600.00
Advanced Nuclear	\$46,393,836.00	\$46,393,836.00	\$46,393,836.00	\$46,393,836.00
Wind	\$10,871,071.88	\$10,871,071.88	\$10,871,071.88	\$10,871,071.88
Advanced Combustion Turbine	\$16,788,788.30	\$16,788,788.30	\$16,788,788.30	\$16,788,788.30
Solid Oxide Fuel Cell	-	\$21,030,156.92	-	\$21,030,156.92
Hybridized Capital Cost	\$208,299,756.96	\$208,299,756.96	\$182,262,287.34	\$182,262,287.34
\$15/Metric ton CO2	\$330,364,936.49	\$303,572,599.47	\$330,364,936.49	\$303,572,599.47
\$30/Metric ton CO2	\$660,729,872.99	\$607,145,198.94	\$660,729,872.99	\$607,145,198.94
Total Cost	\$350,331,053.14	\$371,361,210.06	\$324,293,583.52	\$345,323,740.44
Total Cost + \$15 tax	\$680,695,989.63	\$674,933,809.53	\$654,658,520.01	\$648,896,339.91
Total Cost + \$30 tax	\$1,011,060,926.13	\$978,506,409.00	\$985,023,456.51	\$952,468,939.38

-50% Coal System Levelized Cost Comparisons					
Cost Source	Conventional Coal Reference System Levelized Cost (\$)	Hybrid Energy System Levelized Cost No HTSE (\$)	Base Hybrid System Levelized Cost (\$)	10% Hybridization No HTSE (\$)	10% Hybridization (\$)
Conventional Coal	\$254,566,314.41	-	-	-	-
PCFB (Advanced Coal)	-	\$99,391,130.10	\$99,391,130.10	\$33,988,800.00	\$33,988,800.00
Advanced Nuclear	-	\$175,963,872.00	\$175,963,872.00	\$46,393,836.00	\$46,393,836.00
Wind	\$10,871,071.88	\$10,871,071.88	\$10,871,071.88	\$10,871,071.88	\$10,871,071.88
Advanced Combustion Turbine	\$65,479,621.92	\$65,479,621.92	\$65,479,621.92	\$65,479,621.92	\$65,479,621.92
Solid Oxide Fuel Cell	-	-	\$3,034,139.91	-	\$3,034,139.91
Hybridized Capital Cost	-	-	-	\$175,475,129.49	\$175,475,129.49
\$15/Metric ton CO2	\$513,717,476.25	\$165,182,468.25	\$161,328,478.49	\$165,182,468.25	\$161,328,478.49
\$30/Metric ton CO2	\$1,027,434,952.50	\$330,364,936.49	\$322,656,956.98	\$330,364,936.49	\$322,656,956.98
Total Cost	\$330,917,008.21	\$351,705,695.90	\$354,739,835.81	\$332,208,459.29	\$335,242,599.20
Total Cost + \$15 tax	\$844,634,484.46	\$516,888,164.15	\$516,068,314.29	\$497,390,927.54	\$496,571,077.68
Total Cost + \$30 tax	\$1,358,351,960.71	\$682,070,632.39	\$677,396,792.78	\$662,573,395.78	\$657,899,556.17

-50% Coal System Levelized Cost Comparisons				
Cost Source	20% Hybridization No HTSE (\$)	20% Hybridization (\$)	30% Hybridization No HTSE (\$)	30% Hybridization (\$)
Conventional Coal	-	-	-	-
PCFB (Advanced Coal)	\$33,988,800.00	\$33,988,800.00	\$33,988,800.00	\$33,988,800.00
Advanced Nuclear	\$46,393,836.00	\$46,393,836.00	\$46,393,836.00	\$46,393,836.00
Wind	\$10,871,071.88	\$10,871,071.88	\$10,871,071.88	\$10,871,071.88
Advanced Combustion Turbine	\$65,479,621.92	\$65,479,621.92	\$65,479,621.92	\$65,479,621.92
Solid Oxide Fuel Cell	-	\$3,034,139.91	-	\$3,034,139.91
Hybridized Capital Cost	\$155,977,892.88	\$155,977,892.88	\$136,480,656.27	\$136,480,656.27
\$15/Metric ton CO2	\$165,182,468.25	\$161,328,478.49	\$165,182,468.25	\$161,328,478.49
\$30/Metric ton CO2	\$330,364,936.49	\$322,656,956.98	\$330,364,936.49	\$322,656,956.98
Total Cost	\$312,711,222.68	\$315,745,362.59	\$293,213,986.07	\$296,248,125.98
Total Cost + \$15 tax	\$477,893,690.93	\$477,073,841.07	\$458,396,454.32	\$457,576,604.46
Total Cost + \$30 tax	\$643,076,159.18	\$638,402,319.56	\$623,578,922.57	\$618,905,082.95



+50% Coal System Levelized Cost Comparisons					
Cost Source	Conventional Coal Reference System Levelized Cost (\$)	Hybrid Energy System Levelized Cost No HTSE (\$)	Base Hybrid System Levelized Cost (\$)	10% Hybridization No HTSE (\$)	10% Hybridization (\$)
Conventional Coal	\$418,274,555.18	-	-	-	-
PCFB (Advanced Coal)	-	\$298,173,390.29	\$298,173,390.29	\$101,966,400.00	\$101,966,400.00
Advanced Nuclear	-	\$175,963,872.00	\$175,963,872.00	\$46,393,836.00	\$46,393,836.00
Wind	\$10,871,071.88	\$10,871,071.88	\$10,871,071.88	\$10,871,071.88	\$10,871,071.88
Advanced Combustion Turbine	\$3,247,091.35	\$3,247,091.35	\$3,247,091.35	\$3,247,091.35	\$3,247,091.35
Solid Oxide Fuel Cell	-	-	\$51,645,987.15	-	\$51,645,987.15
Hybridized Capital Cost	-	-	-	\$293,199,323.66	\$293,199,323.66
\$15/Metric ton CO2	\$844,082,412.74	\$495,547,404.74	\$429,719,741.09	\$495,547,404.74	\$429,719,741.09
\$30/Metric ton CO2	\$1,688,164,825.49	\$991,094,809.48	\$859,439,482.18	\$991,094,809.48	\$859,439,482.18
Total Cost	\$432,392,718.42	\$488,255,425.52	\$539,901,412.67	\$455,677,722.89	\$507,323,710.05
Total Cost + \$15 tax	\$1,276,475,131.16	\$983,802,830.26	\$969,621,153.77	\$951,225,127.63	\$937,043,451.14
Total Cost + \$30 tax	\$2,120,557,543.90	\$1,479,350,235.01	\$1,399,340,894.86	\$1,446,772,532.38	\$1,366,763,192.23

+50% Coal System Levelized Cost Comparisons				
Cost Source	20% Hybridization No HTSE (\$)	20% Hybridization (\$)	30% Hybridization No HTSE (\$)	30% Hybridization (\$)
Conventional Coal	-	-	-	-
PCFB (Advanced Coal)	\$101,966,400.00	\$101,966,400.00	\$101,966,400.00	\$101,966,400.00
Advanced Nuclear	\$46,393,836.00	\$46,393,836.00	\$46,393,836.00	\$46,393,836.00
Wind	\$10,871,071.88	\$10,871,071.88	\$10,871,071.88	\$10,871,071.88
Advanced Combustion Turbine	\$3,247,091.35	\$3,247,091.35	\$3,247,091.35	\$3,247,091.35
Solid Oxide Fuel Cell	-	\$51,645,987.15	-	\$51,645,987.15
Hybridized Capital Cost	\$260,621,621.03	\$260,621,621.03	\$228,043,918.40	\$228,043,918.40
\$15/Metric ton CO2	\$495,547,404.74	\$429,719,741.09	\$495,547,404.74	\$429,719,741.09
\$30/Metric ton CO2	\$991,094,809.48	\$859,439,482.18	\$991,094,809.48	\$859,439,482.18
Total Cost	\$423,100,020.26	\$474,746,007.42	\$390,522,317.63	\$442,168,304.79
Total Cost + \$15 tax	\$918,647,425.01	\$904,465,748.51	\$886,069,722.38	\$871,888,045.88
Total Cost + \$30 tax	\$1,414,194,829.75	\$1,334,185,489.60	\$1,381,617,127.12	\$1,301,607,786.97

Double Nuclear System Levelized Cost Comparisons					
Cost Source	Conventional Coal Reference System Levelized Cost (\$)	Hybrid Energy System Levelized Cost No HTSE (\$)	Base Hybrid System Levelized Cost (\$)	10% Hybridization No HTSE (\$)	10% Hybridization (\$)
Conventional Coal	\$509,132,628.82	-	-	-	-
PCFB (Advanced Coal)	-	\$198,782,260.19	\$198,782,260.19	\$67,977,600.00	\$67,977,600.00
Advanced Nuclear	-	\$351,927,744.00	\$351,927,744.00	\$92,787,672.00	\$92,787,672.00
Wind	\$10,871,071.88	\$10,871,071.88	\$10,871,071.88	\$10,871,071.88	\$10,871,071.88
Advanced Combustion Turbine	\$31,852.32	\$31,852.32	\$31,852.32	\$31,852.32	\$31,852.32
Solid Oxide Fuel Cell	-	-	\$89,871,946.71	-	\$89,871,946.71
Hybridized Capital Cost	-	-	-	\$350,950,258.97	\$350,950,258.97
\$15/Metric ton CO2	\$1,027,434,952.50	\$330,364,936.49	\$215,762,673.08	\$330,364,936.49	\$215,762,673.08
\$30/Metric ton CO2	\$2,054,869,905.00	\$660,729,872.99	\$431,525,346.17	\$660,729,872.99	\$431,525,346.17
Total Cost	\$520,035,553.02	\$561,612,928.40	\$651,484,875.11	\$522,618,455.18	\$612,490,401.89
Total Cost + \$15 tax	\$1,547,470,505.51	\$891,977,864.89	\$867,247,548.19	\$852,983,391.67	\$828,253,074.97
Total Cost + \$30 tax	\$2,574,905,458.01	\$1,222,342,801.38	\$1,083,010,221.27	\$1,183,348,328.16	\$1,044,015,748.06

Double Nuclear System Levelized Cost Comparisons				
Cost Source	20% Hybridization No HTSE (\$)	20% Hybridization (\$)	30% Hybridization No HTSE (\$)	30% Hybridization (\$)
Conventional Coal	-	-	-	-
PCFB (Advanced Coal)	\$67,977,600.00	\$67,977,600.00	\$67,977,600.00	\$67,977,600.00
Advanced Nuclear	\$92,787,672.00	\$92,787,672.00	\$92,787,672.00	\$92,787,672.00
Wind	\$10,871,071.88	\$10,871,071.88	\$10,871,071.88	\$10,871,071.88
Advanced Combustion Turbine	\$31,852.32	\$31,852.32	\$31,852.32	\$31,852.32
Solid Oxide Fuel Cell	-	\$89,871,946.71	-	\$89,871,946.71
Hybridized Capital Cost	\$311,955,785.76	\$311,955,785.76	\$272,961,312.54	\$272,961,312.54
\$15/Metric ton CO2	\$330,364,936.49	\$215,762,673.08	\$330,364,936.49	\$215,762,673.08
\$30/Metric ton CO2	\$660,729,872.99	\$431,525,346.17	\$660,729,872.99	\$431,525,346.17
Total Cost	\$483,623,981.96	\$573,495,928.67	\$444,629,508.74	\$534,501,455.45
Total Cost + \$15 tax	\$813,988,918.45	\$789,258,601.75	\$774,994,445.23	\$750,264,128.53
Total Cost + \$30 tax	\$1,144,353,854.95	\$1,005,021,274.84	\$1,105,359,381.73	\$966,026,801.62

-50% Wind System Levelized Cost Comparisons					
Cost Source	Conventional Coal Reference System Levelized Cost (\$)	Hybrid Energy System Levelized Cost No HTSE (\$)	Base Hybrid System Levelized Cost (\$)	10% Hybridization No HTSE (\$)	10% Hybridization (\$)
Conventional Coal	\$336,420,434.80	-	-	-	-
PCFB (Advanced Coal)	-	\$198,782,260.19	\$198,782,260.19	\$67,977,600.00	\$67,977,600.00
Advanced Nuclear	-	\$175,963,872.00	\$175,963,872.00	\$46,393,836.00	\$46,393,836.00
Wind	\$5,435,535.94	\$5,435,535.94	\$5,435,535.94	\$5,435,535.94	\$5,435,535.94
Advanced Combustion Turbine	\$17,764,135.76	\$17,764,135.76	\$17,764,135.76	\$17,764,135.76	\$17,764,135.76
Solid Oxide Fuel Cell	-	-	\$18,389,630.35	-	\$18,389,630.35
Hybridized Capital Cost	-	-	-	\$234,337,226.57	\$234,337,226.57
\$15/Metric ton CO2	\$678,899,944.50	\$330,364,936.49	\$306,940,676.40	\$330,364,936.49	\$306,940,676.40
\$30/Metric ton CO2	\$1,357,799,888.99	\$660,729,872.99	\$613,881,352.80	\$660,729,872.99	\$613,881,352.80
Total Cost	\$359,620,106.49	\$397,945,803.89	\$416,335,434.24	\$371,908,334.27	\$390,297,964.62
Total Cost + \$15 tax	\$1,038,520,050.99	\$728,310,740.39	\$723,276,110.64	\$702,273,270.77	\$697,238,641.02
Total Cost + \$30 tax	\$1,717,419,995.49	\$1,058,675,676.88	\$1,030,216,787.04	\$1,032,638,207.26	\$1,004,179,317.42

-50% Wind System Levelized Cost Comparisons				
Cost Source	20% Hybridization No HTSE (\$)	20% Hybridization (\$)	30% Hybridization No HTSE (\$)	30% Hybridization (\$)
Conventional Coal	-	-	-	-
PCFB (Advanced Coal)	\$67,977,600.00	\$67,977,600.00	\$67,977,600.00	\$67,977,600.00
Advanced Nuclear	\$46,393,836.00	\$46,393,836.00	\$46,393,836.00	\$46,393,836.00
Wind	\$5,435,535.94	\$5,435,535.94	\$5,435,535.94	\$5,435,535.94
Advanced Combustion Turbine	\$17,764,135.76	\$17,764,135.76	\$17,764,135.76	\$17,764,135.76
Solid Oxide Fuel Cell	-	\$18,389,630.35	-	\$18,389,630.35
Hybridized Capital Cost	\$208,299,756.96	\$208,299,756.96	\$182,262,287.34	\$182,262,287.34
\$15/Metric ton CO2	\$330,364,936.49	\$306,940,676.40	\$330,364,936.49	\$306,940,676.40
\$30/Metric ton CO2	\$660,729,872.99	\$613,881,352.80	\$660,729,872.99	\$613,881,352.80
Total Cost	\$345,870,864.65	\$364,260,495.00	\$319,833,395.03	\$338,223,025.38
Total Cost + \$15 tax	\$676,235,801.15	\$671,201,171.40	\$650,198,331.53	\$645,163,701.78
Total Cost + \$30 tax	\$1,006,600,737.64	\$978,141,847.80	\$980,563,268.02	\$952,104,378.18

+50% Wind System Levelized Cost Comparisons					
Cost Source	Conventional Coal Reference System Levelized Cost (\$)	Hybrid Energy System Levelized Cost No HTSE (\$)	Base Hybrid System Levelized Cost (\$)	10% Hybridization No HTSE (\$)	10% Hybridization (\$)
Conventional Coal	\$336,420,434.80	-	-	-	-
PCFB (Advanced Coal)	-	\$198,782,260.19	\$198,782,260.19	\$67,977,600.00	\$67,977,600.00
Advanced Nuclear	-	\$175,963,872.00	\$175,963,872.00	\$46,393,836.00	\$46,393,836.00
Wind	\$16,306,607.82	\$16,306,607.82	\$16,306,607.82	\$16,306,607.82	\$16,306,607.82
Advanced Combustion Turbine	\$16,002,201.99	\$16,002,201.99	\$16,002,201.99	\$16,002,201.99	\$16,002,201.99
Solid Oxide Fuel Cell	-	-	\$23,738,455.58	-	\$23,738,455.58
Hybridized Capital Cost	-	-	-	\$234,337,226.57	\$234,337,226.57
\$15/Metric ton CO2	\$678,899,944.50	\$330,364,936.49	\$300,118,077.06	\$330,364,936.49	\$300,118,077.06
\$30/Metric ton CO2	\$1,357,799,888.99	\$660,729,872.99	\$600,236,154.12	\$660,729,872.99	\$600,236,154.12
Total Cost	\$368,729,244.60	\$407,054,942.00	\$430,793,397.58	\$381,017,472.38	\$404,755,927.96
Total Cost + \$15 tax	\$1,047,629,189.10	\$737,419,878.50	\$730,911,474.64	\$711,382,408.88	\$704,874,005.02
Total Cost + \$30 tax	\$1,726,529,133.60	\$1,067,784,814.99	\$1,031,029,551.70	\$1,041,747,345.37	\$1,004,992,082.08

+50% Wind System Levelized Cost Comparisons				
Cost Source	20% Hybridization No HTSE (\$)	20% Hybridization (\$)	30% Hybridization No HTSE (\$)	30% Hybridization (\$)
Conventional Coal	-	-	-	-
PCFB (Advanced Coal)	\$67,977,600.00	\$67,977,600.00	\$67,977,600.00	\$67,977,600.00
Advanced Nuclear	\$46,393,836.00	\$46,393,836.00	\$46,393,836.00	\$46,393,836.00
Wind	\$16,306,607.82	\$16,306,607.82	\$16,306,607.82	\$16,306,607.82
Advanced Combustion Turbine	\$16,002,201.99	\$16,002,201.99	\$16,002,201.99	\$16,002,201.99
Solid Oxide Fuel Cell	-	\$23,738,455.58	-	\$23,738,455.58
Hybridized Capital Cost	\$208,299,756.96	\$208,299,756.96	\$182,262,287.34	\$182,262,287.34
\$15/Metric ton CO2	\$330,364,936.49	\$300,118,077.06	\$330,364,936.49	\$300,118,077.06
\$30/Metric ton CO2	\$660,729,872.99	\$600,236,154.12	\$660,729,872.99	\$600,236,154.12
Total Cost	\$354,980,002.76	\$378,718,458.34	\$328,942,533.14	\$352,680,988.72
Total Cost + \$15 tax	\$685,344,939.26	\$678,836,535.40	\$659,307,469.64	\$652,799,065.78
Total Cost + \$30 tax	\$1,015,709,875.75	\$978,954,612.46	\$989,672,406.13	\$952,917,142.84



	Value of Syngas Produced to Match Conventional Coal Cost for Base System			
	Base Hybrid System (\$)	10% Hybridization (\$)	20% Hybridization (\$)	30% Hybridization (\$)
No Tax	\$59,355,854.32	\$33,318,384.70	\$7,280,915.08	-\$18,756,554.54
\$15/Metric ton CO <sub>2</sub>	-\$315,971,490.71	-\$342,008,960.33	-\$368,046,429.95	-\$394,083,899.56
\$30/Metric ton CO <sub>2</sub>	-\$691,298,835.73	-\$717,336,305.35	-\$743,373,774.97	-\$769,411,244.59

	Syngas Sale Price to Match Conventional Coal Cost for Base System			
	Base Hybrid System (\$/1000 SCF)	10% Hybridization (\$/1000 SCF)	20% Hybridization (\$/1000 SCF)	30% Hybridization (\$/1000 SCF)
No Tax	\$0.63	\$0.36	\$0.08	Profitable at any
\$15/Metric ton CO <sub>2</sub>	Profitable at any	Profitable at any	Profitable at any	Profitable at any
\$30/Metric ton CO <sub>2</sub>	Profitable at any	Profitable at any	Profitable at any	Profitable at any

	Value of Syngas Produced to Match Conventional Coal Cost for -50% Coal System			
	Base Hybrid System (\$)	10% Hybridization (\$)	20% Hybridization (\$)	30% Hybridization (\$)
No Tax	\$23,822,827.59	\$4,325,590.98	-\$15,171,645.62	-\$34,668,882.23
\$15/Metric ton CO2	-\$328,566,170.17	-\$348,063,406.78	-\$367,560,643.39	-\$387,057,880.00
\$30/Metric ton CO2	-\$680,955,167.93	-\$700,452,404.54	-\$719,949,641.15	-\$739,446,877.76

	Syngas Sale Price to Match Conventional Coal Cost for -50% Coal System			
	Base Hybrid System (\$/1000 SCF)	10% Hybridization (\$/1000 SCF)	20% Hybridization (\$/1000 SCF)	30% Hybridization (\$/1000 SCF)
No Tax	\$1.77	\$0.32	Profitable at any	Profitable at any
\$15/Metric ton CO2	Profitable at any	Profitable at any	Profitable at any	Profitable at any
\$30/Metric ton CO2	Profitable at any	Profitable at any	Profitable at any	Profitable at any

	Value of Syngas Produced to Match Conventional Coal Cost for +50% Coal System			
	Base Hybrid System (\$)	10% Hybridization (\$)	20% Hybridization (\$)	30% Hybridization (\$)
No Tax	\$107,508,694.26	\$74,930,991.63	\$42,353,289.00	\$9,775,586.37
\$15/Metric ton CO <sub>2</sub>	-\$306,853,977.39	-\$339,431,680.02	-\$372,009,382.65	-\$404,587,085.28
\$30/Metric ton CO <sub>2</sub>	-\$721,216,649.04	-\$753,794,351.67	-\$786,372,054.30	-\$818,949,756.93

	Syngas Sale Price to Match Conventional Coal Cost for +50% Coal System			
	Base Hybrid System (\$/1000 SCF)	10% Hybridization (\$/1000 SCF)	20% Hybridization (\$/1000 SCF)	30% Hybridization (\$/1000 SCF)
No Tax	\$0.47	\$0.33	\$0.18	\$0.04
\$15/Metric ton CO <sub>2</sub>	Profitable at any	Profitable at any	Profitable at any	Profitable at any
\$30/Metric ton CO <sub>2</sub>	Profitable at any	Profitable at any	Profitable at any	Profitable at any

	Value of Syngas Produced to Match Conventional Coal Cost for Double Nuclear			
	Base Hybrid System (\$)	10% Hybridization (\$)	20% Hybridization (\$)	30% Hybridization (\$)
No Tax	\$131,449,322.09	\$92,454,848.87	\$53,460,375.65	\$14,465,902.43
\$15/Metric ton CO2	-\$680,222,957.32	-\$719,217,430.54	-\$758,211,903.76	-\$797,206,376.98
\$30/Metric ton CO2	-\$1,491,895,236.74	-\$1,530,889,709.96	-\$1,569,884,183.18	-\$1,608,878,656.40

	Syngas Sale Price to Match Conventional Coal Cost for Double Nuclear			
	Base Hybrid System (\$/1000 SCF)	10% Hybridization (\$/1000 SCF)	20% Hybridization (\$/1000 SCF)	30% Hybridization (\$/1000 SCF)
No Tax	\$0.33	\$0.23	\$0.13	\$0.04
\$15/Metric ton CO2	Profitable at any	Profitable at any	Profitable at any	Profitable at any
\$30/Metric ton CO2	Profitable at any	Profitable at any	Profitable at any	Profitable at any

	Value of Syngas Produced to Match Conventional Coal Cost for -50% Wind System			
	Base Hybrid System (\$)	10% Hybridization (\$)	20% Hybridization (\$)	30% Hybridization (\$)
No Tax	\$56,715,327.75	\$30,677,858.13	\$4,640,388.51	-\$21,397,081.11
\$15/Metric ton CO <sub>2</sub>	-\$315,243,940.35	-\$341,281,409.97	-\$367,318,879.59	-\$393,356,349.21
\$30/Metric ton CO <sub>2</sub>	-\$687,203,208.45	-\$713,240,678.07	-\$739,278,147.69	-\$765,315,617.31

	Syngas Sale Price to Match Conventional Coal Cost -50% Wind System			
	Base Hybrid System (\$/1000 SCF)	10% Hybridization (\$/1000 SCF)	20% Hybridization (\$/1000 SCF)	30% Hybridization (\$/1000 SCF)
No Tax	\$0.69	\$0.38	\$0.06	Profitable at any
\$15/Metric ton CO <sub>2</sub>	Profitable at any	Profitable at any	Profitable at any	Profitable at any
\$30/Metric ton CO <sub>2</sub>	Profitable at any	Profitable at any	Profitable at any	Profitable at any

	Value of Syngas Produced to Match Conventional Coal Cost for +50% Wind System			
	Base Hybrid System (\$)	10% Hybridization (\$)	20% Hybridization (\$)	30% Hybridization (\$)
No Tax	\$62,064,152.97	\$36,026,683.35	\$9,989,213.74	-\$16,048,255.88
\$15/Metric ton CO2	-\$316,717,714.46	-\$342,755,184.08	-\$368,792,653.70	-\$394,830,123.32
\$30/Metric ton CO2	-\$695,499,581.90	-\$721,537,051.52	-\$747,574,521.13	-\$773,611,990.75

	Syngas Sale Price to Match Conventional Coal Cost +50% Wind System			
	Base Hybrid System (\$/1000 SCF)	10% Hybridization (\$/1000 SCF)	20% Hybridization (\$/1000 SCF)	30% Hybridization (\$/1000 SCF)
No Tax	\$0.59	\$0.34	\$0.09	Profitable at any
\$15/Metric ton CO2	Profitable at any	Profitable at any	Profitable at any	Profitable at any
\$30/Metric ton CO2	Profitable at any	Profitable at any	Profitable at any	Profitable at any

## SECTION

### 2. CONCLUSIONS

This work has outlined the model framework for a modular hybrid energy system. The approach allows for ease of future modification of unit systems and integration of new model units. This work demonstrates how a hybrid system can be modeled and feasibly integrated. The issue of grid stability arising from the use of large scale renewables is addressed with the sustainable hybrid energy system.

While society may wish for carbon free electricity, it also maintains itself on the availability of instantaneous and cheap power as well. The hybrid system is the economical stepping stone to reach that goal. This system allows for the cheap electricity society demands while simultaneously reducing carbon emissions and bringing larger scale renewables online.

This work is the first novel solution that utilizes the carbon dioxide emitted by turning a potential pollutant into another chemical feedstock. The value added by chemical production makes the hybrid system cost competitive and economically viable when compared to other conventional generation sources.

Future work can build upon this model to introduce other generation sources such as biomass, solar, geothermal, hydroelectric, etc. Additional work can also be done in the area of hybridized cost reduction to see the true value that hybridizing systems can bring. If a model hierarchy can be constructed for producing synfuel from syngas, such as through Fischer-Tropsch reactions, it can be easily inserted into the Aspen Plus model framework.

## **APPENDIX A.**

### **RIGOROUS STEADY STATE ASPEN PLUS INPUT**



The following script is the input file that will generate an Aspen Plus simulation used in this work. This script will generate the steady state model that rigorously simulates the hybrid coal and nuclear system with HTSE and enriched oxygen air recycle:

```
;
;Input Summary created by Aspen Plus Rel. 25.0 at 10:40:18 Wed Jul 15, 2015
;Directory Filename C:\Users\klbtz3\Desktop\HES Research Main\HES model
dynamic\Integrated HES w_design changes\Changing number of cells\hes model 100.inp
;
```

#### DYNAMICS

DYNAMICS RESULTS=ON

IN-UNITS ENG ENTHALPY-FLO=kW

DEF-STREAMS CONVEN ALL

SIM-OPTIONS MASS-BAL-CHE=YES FLASH-MAXIT=40 BYPASS-PROP=NO &  
FLASH-METHOD=GIBBS OPER-YEAR=365. <day>

DATABANKS 'APV73 PURE25' / 'APV73 AQUEOUS' / 'APV73 SOLIDS' / &  
'APV73 INORGANIC' / 'APV73 COMBUST' / 'APV73 PURE20' / &  
'APV73 ASPENPCD'

PROP-SOURCES 'APV73 PURE25' / 'APV73 AQUEOUS' / 'APV73 SOLIDS' &  
/ 'APV73 INORGANIC' / 'APV73 COMBUST' / 'APV73 PURE20' &  
/ 'APV73 ASPENPCD'

#### COMPONENTS

WATER H2O /  
CO2 CO2 /  
CO CO /  
N2 N2 /  
H2 H2 /  
CH4 CH4 /  
O2 O2 /  
ARGON AR /  
CARBON C /  
SULFUR S /  
NO2 NO2 /  
NO NO /

HCL HCL /  
 CL2 CL2 /  
 SO2 O2S /  
 H2O H2O /  
 AR AR /  
 C2H4 C2H4 /  
 C2H2 C2H2 /  
 C2H6 C2H6 /  
 C3H8 C3H8 /  
 H3N H3N /  
 N2O N2O /  
 O2S O2S /  
 O3S O3S /  
 H2S H2S /  
 NITRO-01 N2 /  
 OXYGE-01 O2

HENRY-COMPS HC-1 CO2

#### FLOWSHEET

HIERARCHY HTSE  
 CONNECT \$C-3 IN=CO2HTSE OUT="HTSE.CO2HTSE"  
 CONNECT \$C-6 IN=NUCSTEAM OUT="HTSE.NUCSTEAM"  
 CONNECT \$C-4 IN="HTSE.ENR-AIR" OUT=ENR-AIR  
 CONNECT \$C-7 IN="HTSE.SYNGAS-2" OUT=SYNGAS  
 CONNECT \$C-9 IN="HTSE.1" OUT=CO2-XTRA  
 HIERARCHY PCFB  
 CONNECT \$C-1 IN=COALAIR OUT="PCFB.11"  
 CONNECT \$C-2 IN=COALAIR2 OUT="PCFB.COALAIR2"  
 CONNECT \$C-5 IN="PCFB.RELEASE" OUT=EFFLUENT  
 HIERARCHY SMR  
 CONNECT \$C-8 IN="SMR.7" OUT=NUCSTEAM  
 BLOCK AIR-SPLT IN=1 ENR-AIR OUT=COALAIR2 COALAIR  
 BLOCK B3 IN=AIR OUT=1  
 BLOCK CO2SEP IN=EFFLUENT OUT=CO2HTSE 2

#### PROPERTIES PR-BM

PROPERTIES ELECNRTL / IAPWS-95 / IDEAL / PENG-ROB /  
 RKS-BM / WILSON

#### PROP-DATA REVIEW-1

IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr' &  
 HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=C &  
 VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum' &  
 MASS-DENSITY='kg/cum' MOLE-ENTHALP='kcal/mol' &  
 MASS-ENTHALP='kcal/kg' HEAT=Gcal MOLE-CONC='mol/l' &

```

PDROP=bar
PROP-LIST API / DGFORM / DGSFRM / DHFORM / DHSFRM / &
  DHVLB / FREEZEPT / HCOM / MUP / MW / OMEGA / PC / &
  RKTZRA / SG / TB / TC / VB / VC / VLSTD / ZC
PVAL H2O 10.0 / -54.6343 / -56.5492 / -57.7949 / &
  -69.9627 / 9.744507 / 0.0 / 0.0 / 1.84972 / &
  18.01528 / 0.344861 / 220.64 / 0.243172 / 1.0 / &
  100.0 / 373.946 / 18.8311 / 55.9472 / 18.0691 / &
  0.229
PROP-LIST DHFORM / FREEZEPT / MW / PC / VC / VLSTD / &
  ZC / RGYR
PVAL CO2 -94.05110000 / -56.57 / 44.0095 / 73.83 / 94 / &
  61.6782 / 0.274 / 1.04000E-10

PROP-DATA CPDIEC-1
IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr' &
  HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=C &
  VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum' &
  MASS-DENSITY='kg/cum' MOLE-ENTHALP='kcal/mol' &
  MASS-ENTHALP='kcal/kg' HEAT=Gcal MOLE-CONC='mol/l' &
  PDROP=bar
PROP-LIST CPDIEC
PVAL H2O 78.24662286 32730.85746 298.15

PROP-DATA DHVLWT-1
IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr' &
  HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=C &
  VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum' &
  MASS-DENSITY='kg/cum' MOLE-ENTHALP='J/kmol' &
  MASS-ENTHALP='kcal/kg' HEAT=Gcal MOLE-CONC='mol/l' &
  PDROP=bar
PROP-LIST DHVLWT
PVAL H2O 40655000 100.00 0.26623503 0.09110321 0.01

PROP-DATA HENRY-1
IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr' &
  HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=Pa TEMPERATURE=K &
  VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum' &
  MASS-DENSITY='kg/cum' MOLE-ENTHALP='kcal/mol' &
  MASS-ENTHALP='kcal/kg' HEAT=Gcal MOLE-CONC='mol/l' &
  PDROP=bar
PROP-LIST HENRY
BPVAL CO2 H2O 170.7126000 -8477.711000 -21.95743000 &
  5.78074800E-3 273.0000000 500.0000000 0.0

PROP-DATA HENRY-1

```

IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr' &  
 HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=C &  
 VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum' &  
 MASS-DENSITY='kg/cum' MOLE-ENTHALP='kcal/mol' &  
 MASS-ENTHALP='kcal/kg' HEAT=Gcal MOLE-CONC='mol/l' &  
 PDROP=bar  
 PROP-LIST HENRY  
 BPVAL CO2 WATER 159.8650745 -8741.550000 -21.66900000 &  
 1.10259000E-3 -.1500000000 79.85000000 0.0

# PROP-DATA NRTL-1

IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr' &  
 HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=C &  
 VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum' &  
 MASS-DENSITY='kg/cum' MOLE-ENTHALP='kcal/mol' &  
 MASS-ENTHALP='kcal/kg' HEAT=Gcal MOLE-CONC='mol/l' &  
 PDROP=bar  
 PROP-LIST NRTL  
 BPVAL H2O CO2 10.06400000 -3268.135000 .2000000000 0.0 0.0 &  
 0.0 0.0 200.0000000  
 BPVAL CO2 H2O 10.06400000 -3268.135000 .2000000000 0.0 0.0 &  
 0.0 0.0 200.0000000  
 BPVAL WATER CO2 10.06400000 -3268.135000 .2000000000 0.0 &  
 0.0 0.0 0.0 200.0000000  
 BPVAL CO2 WATER 10.06400000 -3268.135000 .2000000000 0.0 &  
 0.0 0.0 0.0 200.0000000  
 BPVAL WATER H3N -.5440720000 1678.469000 .2000000000 0.0 &  
 0.0 0.0 0.0 200.0000000  
 BPVAL H3N WATER -.1642422000 -1027.525000 .2000000000 0.0 &  
 0.0 0.0 0.0 200.0000000  
 BPVAL WATER H2S -3.674000000 1155.900000 .2000000000 0.0 &  
 0.0 0.0 0.0 150.0000000  
 BPVAL H2S WATER -3.674000000 1155.900000 .2000000000 0.0 &  
 0.0 0.0 0.0 150.0000000  
 BPVAL H2O H3N -.5440720000 1678.469000 .2000000000 0.0 0.0 &  
 0.0 0.0 200.0000000  
 BPVAL H3N H2O -.1642422000 -1027.525000 .2000000000 0.0 &  
 0.0 0.0 0.0 200.0000000  
 BPVAL H2O H2S -3.674000000 1155.900000 .2000000000 0.0 0.0 &  
 0.0 0.0 150.0000000  
 BPVAL H2S H2O -3.674000000 1155.900000 .2000000000 0.0 0.0 &  
 0.0 0.0 150.0000000

# PROP-DATA RKSKBV-1

IN-UNITS SI  
 PROP-LIST RKSKBV

BPVAL WATER CO2 .0737000000 0.0 0.0 0.0 1000.000000  
 BPVAL CO2 WATER .0737000000 0.0 0.0 0.0 1000.000000  
 BPVAL CO2 N2 -.0315000000 0.0 0.0 0.0 1000.000000  
 BPVAL N2 CO2 -.0315000000 0.0 0.0 0.0 1000.000000  
 BPVAL CO2 H2 -.3426000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2 CO2 -.3426000000 0.0 0.0 0.0 1000.000000  
 BPVAL CO2 CH4 .0933000000 0.0 0.0 0.0 1000.000000  
 BPVAL CH4 CO2 .0933000000 0.0 0.0 0.0 1000.000000  
 BPVAL CO N2 .0374000000 0.0 0.0 0.0 1000.000000  
 BPVAL N2 CO .0374000000 0.0 0.0 0.0 1000.000000  
 BPVAL CO H2 .0804000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2 CO .0804000000 0.0 0.0 0.0 1000.000000  
 BPVAL CO CH4 .0322000000 0.0 0.0 0.0 1000.000000  
 BPVAL CH4 CO .0322000000 0.0 0.0 0.0 1000.000000  
 BPVAL N2 H2 .0978000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2 N2 .0978000000 0.0 0.0 0.0 1000.000000  
 BPVAL N2 CH4 .0278000000 0.0 0.0 0.0 1000.000000  
 BPVAL CH4 N2 .0278000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2 CH4 -.0222000000 0.0 0.0 0.0 1000.000000  
 BPVAL CH4 H2 -.0222000000 0.0 0.0 0.0 1000.000000  
 BPVAL N2 O2 -7.8000000E-3 0.0 0.0 0.0 1000.000000  
 BPVAL O2 N2 -7.8000000E-3 0.0 0.0 0.0 1000.000000  
 BPVAL N2 ARGON 0.0 0.0 0.0 0.0 1000.000000  
 BPVAL ARGON N2 0.0 0.0 0.0 0.0 1000.000000  
 BPVAL CH4 ARGON .0252000000 0.0 0.0 0.0 1000.000000  
 BPVAL ARGON CH4 .0252000000 0.0 0.0 0.0 1000.000000  
 BPVAL O2 ARGON .0178000000 0.0 0.0 0.0 1000.000000  
 BPVAL ARGON O2 .0178000000 0.0 0.0 0.0 1000.000000  
 BPVAL N2 SO2 .0578000000 0.0 0.0 0.0 1000.000000  
 BPVAL SO2 N2 .0578000000 0.0 0.0 0.0 1000.000000  
 BPVAL CH4 SO2 .1279000000 0.0 0.0 0.0 1000.000000  
 BPVAL SO2 CH4 .1279000000 0.0 0.0 0.0 1000.000000  
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 BPVAL H2O CO2 .0737000000 0.0 0.0 0.0 1000.000000  
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 BPVAL C2H4 CO2 .0533000000 0.0 0.0 0.0 1000.000000  
 BPVAL N2 AR 0.0 0.0 0.0 0.0 1000.000000  
 BPVAL AR N2 0.0 0.0 0.0 0.0 1000.000000  
 BPVAL N2 C2H4 .0798000000 0.0 0.0 0.0 1000.000000  
 BPVAL C2H4 N2 .0798000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2 C2H4 -.0681000000 0.0 0.0 0.0 1000.000000  
 BPVAL C2H4 H2 -.0681000000 0.0 0.0 0.0 1000.000000  
 BPVAL CH4 AR .0252000000 0.0 0.0 0.0 1000.000000  
 BPVAL AR CH4 .0252000000 0.0 0.0 0.0 1000.000000  
 BPVAL CH4 C2H4 .0189000000 0.0 0.0 0.0 1000.000000  
 BPVAL C2H4 CH4 .0189000000 0.0 0.0 0.0 1000.000000

BPVAL O2 AR .0178000000 0.0 0.0 0.0 1000.000000  
 BPVAL AR O2 .0178000000 0.0 0.0 0.0 1000.000000  
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 BPVAL C2H2 C2H4 .0596000000 0.0 0.0 0.0 1000.000000  
 BPVAL CO2 C2H6 .1363000000 0.0 0.0 0.0 1000.000000  
 BPVAL C2H6 CO2 .1363000000 0.0 0.0 0.0 1000.000000  
 BPVAL CO C2H6 -.0278000000 0.0 0.0 0.0 1000.000000  
 BPVAL C2H6 CO -.0278000000 0.0 0.0 0.0 1000.000000  
 BPVAL N2 C2H6 .0407000000 0.0 0.0 0.0 1000.000000  
 BPVAL C2H6 N2 .0407000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2 C2H6 -.1667000000 0.0 0.0 0.0 1000.000000  
 BPVAL C2H6 H2 -.1667000000 0.0 0.0 0.0 1000.000000  
 BPVAL CH4 C2H6 -7.80000000E-3 0.0 0.0 0.0 1000.000000  
 BPVAL C2H6 CH4 -7.80000000E-3 0.0 0.0 0.0 1000.000000  
 BPVAL C2H4 C2H6 .0100000000 0.0 0.0 0.0 1000.000000  
 BPVAL C2H6 C2H4 .0100000000 0.0 0.0 0.0 1000.000000  
 BPVAL CO2 C3H8 .1289000000 0.0 0.0 0.0 1000.000000  
 BPVAL C3H8 CO2 .1289000000 0.0 0.0 0.0 1000.000000  
 BPVAL CO C3H8 .0156000000 0.0 0.0 0.0 1000.000000  
 BPVAL C3H8 CO .0156000000 0.0 0.0 0.0 1000.000000  
 BPVAL N2 C3H8 .0763000000 0.0 0.0 0.0 1000.000000  
 BPVAL C3H8 N2 .0763000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2 C3H8 -.2359000000 0.0 0.0 0.0 1000.000000  
 BPVAL C3H8 H2 -.2359000000 0.0 0.0 0.0 1000.000000  
 BPVAL CH4 C3H8 9.00000000E-3 0.0 0.0 0.0 1000.000000  
 BPVAL C3H8 CH4 9.00000000E-3 0.0 0.0 0.0 1000.000000  
 BPVAL C2H6 C3H8 -2.20000000E-3 0.0 0.0 0.0 1000.000000  
 BPVAL C3H8 C2H6 -2.20000000E-3 0.0 0.0 0.0 1000.000000  
 BPVAL WATER H3N -.2800000000 0.0 0.0 0.0 1000.000000  
 BPVAL H3N WATER -.2800000000 0.0 0.0 0.0 1000.000000  
 BPVAL N2 H3N .2222000000 0.0 0.0 0.0 1000.000000  
 BPVAL H3N N2 .2222000000 0.0 0.0 0.0 1000.000000  
 BPVAL ARGON H3N -.2200000000 0.0 0.0 0.0 1000.000000  
 BPVAL H3N ARGON -.2200000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2O H3N -.2800000000 0.0 0.0 0.0 1000.000000  
 BPVAL H3N H2O -.2800000000 0.0 0.0 0.0 1000.000000  
 BPVAL AR H3N -.2200000000 0.0 0.0 0.0 1000.000000  
 BPVAL H3N AR -.2200000000 0.0 0.0 0.0 1000.000000  
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 BPVAL N2O CO2 2.20000000E-3 0.0 0.0 0.0 1000.000000  
 BPVAL N2 N2O -.0110000000 0.0 0.0 0.0 1000.000000  
 BPVAL N2O N2 -.0110000000 0.0 0.0 0.0 1000.000000  
 BPVAL CH4 N2O .0211000000 0.0 0.0 0.0 1000.000000  
 BPVAL N2O CH4 .0211000000 0.0 0.0 0.0 1000.000000  
 BPVAL O2 N2O .0433000000 0.0 0.0 0.0 1000.000000  
 BPVAL N2O O2 .0433000000 0.0 0.0 0.0 1000.000000

BPVAL N2 O2S .0578000000 0.0 0.0 0.0 1000.000000  
 BPVAL O2S N2 .0578000000 0.0 0.0 0.0 1000.000000  
 BPVAL CH4 O2S .1279000000 0.0 0.0 0.0 1000.000000  
 BPVAL O2S CH4 .1279000000 0.0 0.0 0.0 1000.000000  
 BPVAL WATER H2S .0100000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2S WATER .0100000000 0.0 0.0 0.0 1000.000000  
 BPVAL CO2 H2S .0989000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2S CO2 .0989000000 0.0 0.0 0.0 1000.000000  
 BPVAL CO H2S .0367000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2S CO .0367000000 0.0 0.0 0.0 1000.000000  
 BPVAL N2 H2S .1696000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2S N2 .1696000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2O H2S .0100000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2S H2O .0100000000 0.0 0.0 0.0 1000.000000  
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 BPVAL H2S C2H6 .0852000000 0.0 0.0 0.0 1000.000000  
 BPVAL C3H8 H2S .0885000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2S C3H8 .0885000000 0.0 0.0 0.0 1000.000000  
 BPVAL CO2 NITRO-01 -.0315000000 0.0 0.0 0.0 1000.000000  
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 BPVAL NITRO-01 CO .0374000000 0.0 0.0 0.0 1000.000000  
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 BPVAL NITRO-01 H2 .0978000000 0.0 0.0 0.0 1000.000000  
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 BPVAL NITRO-01 ARGON 0.0 0.0 0.0 0.0 1000.000000  
 BPVAL ARGON OXYGE-01 .0178000000 0.0 0.0 0.0 1000.000000  
 BPVAL OXYGE-01 ARGON .0178000000 0.0 0.0 0.0 1000.000000  
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 BPVAL NITRO-01 SO2 .0578000000 0.0 0.0 0.0 1000.000000  
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 BPVAL NITRO-01 AR 0.0 0.0 0.0 0.0 1000.000000  
 BPVAL AR OXYGE-01 .0178000000 0.0 0.0 0.0 1000.000000  
 BPVAL OXYGE-01 AR .0178000000 0.0 0.0 0.0 1000.000000  
 BPVAL C2H4 NITRO-01 .0798000000 0.0 0.0 0.0 1000.000000  
 BPVAL NITRO-01 C2H4 .0798000000 0.0 0.0 0.0 1000.000000  
 BPVAL C2H6 NITRO-01 .0407000000 0.0 0.0 0.0 1000.000000  
 BPVAL NITRO-01 C2H6 .0407000000 0.0 0.0 0.0 1000.000000  
 BPVAL C3H8 NITRO-01 .0763000000 0.0 0.0 0.0 1000.000000  
 BPVAL NITRO-01 C3H8 .0763000000 0.0 0.0 0.0 1000.000000

BPVAL H3N NITRO-01 .2222000000 0.0 0.0 0.0 1000.000000  
 BPVAL NITRO-01 H3N .2222000000 0.0 0.0 0.0 1000.000000  
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 BPVAL OXYGE-01 N2O .0433000000 0.0 0.0 0.0 1000.000000  
 BPVAL O2S NITRO-01 .0578000000 0.0 0.0 0.0 1000.000000  
 BPVAL NITRO-01 O2S .0578000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2S NITRO-01 .1696000000 0.0 0.0 0.0 1000.000000  
 BPVAL NITRO-01 H2S .1696000000 0.0 0.0 0.0 1000.000000  
 BPVAL NITRO-01 OXYGE-01 -7.8000000E-3 0.0 0.0 0.0 &  
 1000.000000  
 BPVAL OXYGE-01 NITRO-01 -7.8000000E-3 0.0 0.0 0.0 &  
 1000.000000

#### PROP-DATA WILSON-1

IN-UNITS ENG ENTHALPY-FLO=kW

PROP-LIST WILSON

BPVAL WATER H3N -7.914400000 4772.888962 0.0 0.0 &  
 50.00000360 196.7000024 0.0  
 BPVAL H3N WATER 5.290700000 -2178.199963 0.0 0.0 &  
 50.00000360 196.7000024 0.0  
 BPVAL H2O H3N -7.914400000 4772.888962 0.0 0.0 50.00000360 &  
 196.7000024 0.0  
 BPVAL H3N H2O 5.290700000 -2178.199963 0.0 0.0 50.00000360 &  
 196.7000024 0.0

#### STREAM 1

SUBSTREAM MIXED TEMP=77 PRES=16.696

MOLE-FLOW N2 17052.8047 / O2 4533.02402

#### STREAM 2

SUBSTREAM MIXED TEMP=1155.84778 PRES=14.696

MOLE-FLOW WATER 3656.91552 / CO2 860.178686 / CO &  
 949.524817 / N2 22617.1042 / H2 342.352181 / CH4 &  
 0.00220356054 / SULFUR 1.703212E-006 / NO &  
 5.769462E-008 / HCL 4.82248014 / CL2 2.420841E-011 / &  
 SO2 0.0877787636 / C2H4 1.471721E-010 / C2H2 &  
 2.861227E-011 / H3N 0.0892413192 / N2O 1.119908E-011 / &  
 O2S 0.0877787636 / O3S 1.057665E-009 / H2S 69.1380203

#### STREAM AIR

SUBSTREAM MIXED TEMP=77 PRES=16.696 MOLE-FLOW=73790.8

MOLE-FRAC N2 0.79 / O2 0.21

#### STREAM CO2-XTRA



SUBSTREAM MIXED TEMP=1155.84778 PRES=14.696  
MOLE-FLOW CO2 4774.43861

#### STREAM CO2HTSE

SUBSTREAM MIXED TEMP=1155.84778 PRES=14.696  
MOLE-FLOW CO2 7741.60817

#### STREAM COALAIR

SUBSTREAM MIXED TEMP=493.622545 PRES=16.696 &  
MOLE-FLOW=16289.4716  
MOLE-FRAC N2 0.692165313 / O2 0.307834687

#### STREAM COALAIR2

SUBSTREAM MIXED TEMP=493.622545 PRES=16.696 &  
MOLE-FLOW=16289.4716  
MOLE-FRAC N2 0.692165313 / O2 0.307834687

#### STREAM EFFLUENT

SUBSTREAM MIXED TEMP=1155.84778 PRES=14.696  
MOLE-FLOW WATER 3656.91552 / CO2 8601.78686 / CO &  
949.524817 / N2 22617.1042 / H2 342.352181 / CH4 &  
0.00220356054 / O2 1.812938E-012 / CARBON &  
4.069317E-025 / SULFUR 1.703212E-006 / NO2 &  
7.462433E-017 / NO 5.769462E-008 / HCL 4.82248014 / &  
CL2 2.420841E-011 / SO2 0.0877787636 / C2H4 &  
1.471721E-010 / C2H2 2.861227E-011 / C2H6 &  
6.789494E-012 / C3H8 7.328582E-020 / H3N 0.0892413192 / &  
N2O 1.119908E-011 / O2S 0.0877787636 / O3S &  
1.057665E-009 / H2S 69.1380203

#### STREAM ENR-AIR

SUBSTREAM MIXED TEMP=1244.6778 PRES=336.63  
MASS-FLOW N2 153995.974 / O2 175862.357

#### STREAM NUCSTEAM

SUBSTREAM MIXED TEMP=935.995817 PRES=14.6959488  
MOLE-FLOW H2O 70977.589

#### STREAM SYNGAS

SUBSTREAM MIXED TEMP=1244.6778 PRES=336.63  
MOLE-FLOW CO2 384.22696 / CO 2582.94261 / H2 5486.30307 / &  
H2O 490.058932

#### BLOCK AIR-SPLT FSPLIT

FRAC COALAIR2 0.5

## BLOCK CO2SEP SEP

FRAC STREAM=CO2HTSE SUBSTREAM=MIXED COMPS=WATER CO2 CO &  
 N2 H2 CH4 O2 ARGON CARBON SULFUR NO2 NO HCL CL2 &  
 SO2 H2O AR C2H4 C2H2 C2H6 C3H8 H3N N2O O2S O3S H2S &  
 NITRO-01 OXYGE-01 FRACS=0. 0.9 0. 0. 0. 0. 0. 0. &  
 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. &  
 0. 0. 0. 0. 0.

## HIERARCHY HTSE

## DEF-STREAMS CONVEN ALL

## SOLVE

PARAM METHOD=SM  
 RUN-MODE MODE=SIM

## FLOWSHEET

HIERARCHY HT-ELECT  
 CONNECT \$C-1 IN=HOT-AIR OUT="HT-ELECT.AIR"  
 CONNECT \$C-2 IN=HTE-FEED OUT="HT-ELECT.FEED-GAS"  
 CONNECT \$C-3 IN=HT-INPUT OUT="HT-ELECT.QPROC"  
 CONNECT \$C-4 IN="HT-ELECT.ENR-AIR" OUT=ENR-AIR  
 CONNECT \$C-5 IN="HT-ELECT.SYNGAS" OUT=SYNGAS-1  
 CONNECT \$C-14 IN="HT-ELECT.ELCPWR" OUT=PWR-REQD  
 BLOCK AIR-HTR IN=AIR-2 OUT=HOT-AIR  
 BLOCK FEED-HTR IN=RECY-GAS WATER-1 CO2-1 OUT=HTE-FEED  
 BLOCK SYN-SPLT IN=SYNGAS-1 OUT=RECY-GAS SYNGAS-2  
 BLOCK CO2-COMP IN=CO2 OUT=CO2-1  
 BLOCK AIR-COMP IN=AIR OUT=AIR-2  
 BLOCK B1 IN=CO2HTSE OUT=CO2 1  
 BLOCK B2 IN=NUCSTEAM OUT=XTRASTM WATER  
 BLOCK B3 IN=WATER OUT=WATER-1

## PROPERTIES PR-BM

PROPERTIES ELECNRTL / IAPWS-95 / IDEAL / PENG-ROB /  
 RKS-BM / WILSON

## STREAM 1

SUBSTREAM MIXED TEMP=1155.84778 PRES=14.696  
 MOLE-FLOW CO2 4774.43861

## STREAM AIR

SUBSTREAM MIXED TEMP=77 PRES=1.0000000027 <atm> &  
 MASS-FLOW=200755.295  
 MOLE-FRAC N2 0.79 / O2 0.21

## STREAM AIR-2

SUBSTREAM MIXED TEMP=372.762308 PRES=336.63  
MOLE-FLOW N2 5497.20969 / O2 1461.28359

## STREAM CO2

SUBSTREAM MIXED TEMP=1155.84778 PRES=14.696  
MOLE-FLOW CO2 2967.16957

## STREAM CO2-1

SUBSTREAM MIXED TEMP=1362.30173 PRES=336.63  
MOLE-FLOW CO2 2967.16957

## STREAM CO2HTSE

SUBSTREAM MIXED TEMP=1155.84778 PRES=14.696  
MOLE-FLOW CO2 7741.60817

## STREAM ENR-AIR

SUBSTREAM MIXED TEMP=1244.6778 PRES=336.63  
MOLE-FLOW N2 5497.20969 / O2 5495.90624

## STREAM HOT-AIR

SUBSTREAM MIXED TEMP=1472 PRES=336.63  
MOLE-FLOW N2 5497.20969 / O2 1461.28359

## STREAM HTE-FEED

SUBSTREAM MIXED TEMP=1472 PRES=336.63  
MOLE-FLOW CO2 3019.30779 / CO 350.496071 / H2 744.471698 / &  
H2O 6042.86124

## STREAM NUCSTEAM

SUBSTREAM MIXED TEMP=935.995817 PRES=14.6959488  
MOLE-FLOW H2O 70977.589

## STREAM RECY-GAS

SUBSTREAM MIXED TEMP=1244.6778 PRES=336.63  
MASS-FLOW CO2 2294.57716 / CO 9817.53515 / H2 1500.76561 / &  
H2O 1198.0025

## STREAM SYNGAS-1

SUBSTREAM MIXED TEMP=1244.6778 PRES=336.63  
MOLE-FLOW CO2 436.365184 / CO 2933.43868 / H2 6230.77476 / &  
H2O 556.558176

## STREAM SYNGAS-2

SUBSTREAM MIXED TEMP=1244.6778 PRES=336.63

MOLE-FLOW CO2 384.22696 / CO 2582.94261 / H2 5486.30307 / &  
H2O 490.058932

STREAM WATER

SUBSTREAM MIXED TEMP=935.995817 PRES=1.0000000027 <atm>  
MOLE-FLOW H2O 5976.362

STREAM WATER-1

SUBSTREAM MIXED TEMP=1486.31538 PRES=336.63  
MOLE-FLOW H2O 5976.362

STREAM XTRASTM

SUBSTREAM MIXED TEMP=935.995817 PRES=14.6959488  
MOLE-FLOW H2O 65001.227

DEF-STREAMS HEAT HT-INPUT

STREAM HT-INPUT

INFO HEAT DUTY=0

DEF-STREAMS HEAT PWR-REQD

STREAM PWR-REQD

INFO HEAT DUTY=-252710.835

BLOCK B1 FSPLIT

MASS-FLOW CO2 130583.649

BLOCK B2 FSPLIT

MOLE-FLOW WATER 5976.362

BLOCK SYN-SPLT FSPLIT

FRAC RECY-GAS 0.119483006

BLOCK AIR-HTR HEATER

PARAM TEMP=1472. PRES=0.

BLOCK FEED-HTR HEATER

PARAM TEMP=1472 PRES=0.

HIERARCHY HT-ELECT

DEF-STREAMS CONVEN ALL

SOLVE

PARAM METHOD=SM  
 RUN-MODE MODE=SIM

# FLWSHEET

BLOCK GSR-1 IN=FEED-GAS OUT=GAS-2  
 BLOCK ISOTELC IN=GAS-2 OUT=GAS-3 E-2  
 BLOCK ELDRDS IN=GAS-3 OUT=O2 GAS-4 E-3  
 BLOCK Q-MIX IN=QPROC E-2 E-3 E-1 E-4 OUT=ELCPWR  
 BLOCK AIR-MIX IN=O2 AIR OUT=AIR-3  
 BLOCK AIR-TEMP IN=AIR-3 OUT=ENR-AIR E-1  
 BLOCK GSR-2 IN=GAS-4 OUT=SYNGAS E-4

PROPERTIES PR-BM FREE-WATER=STEAM-TA SOLU-WATER=3 TRUE-COMPS=YES

PROPERTIES ELECNRTL / IAPWS-95 / IDEAL / PENG-ROB /  
 RKS-BM / WILSON

# STREAM AIR

SUBSTREAM MIXED TEMP=1472 PRES=336.63  
 MOLE-FLOW N2 5497.20969 / O2 1461.28359

# STREAM AIR-3

SUBSTREAM MIXED TEMP=1472.3091 PRES=336.63  
 MOLE-FLOW N2 5497.20969 / O2 5495.90624

# STREAM ENR-AIR

SUBSTREAM MIXED TEMP=1244.6778 PRES=336.63  
 MOLE-FLOW N2 5497.20969 / O2 5495.90624

# STREAM FEED-GAS

SUBSTREAM MIXED TEMP=1472 PRES=336.63  
 MOLE-FLOW CO2 3019.30779 / CO 350.496071 / H2 744.471698 / &  
 H2O 6042.86124

# STREAM GAS-2

SUBSTREAM MIXED TEMP=1469.97076 PRES=336.63  
 MOLE-FLOW CO2 3004.06213 / CO 365.741727 / H2 729.226043 / &  
 H2O 6058.1069

# STREAM GAS-3

SUBSTREAM MIXED TEMP=1472 PRES=507.632082  
 MOLE-FLOW CO 3369.80386 / H2 5794.40922 / O2 4034.62266 / &  
 H2O 992.923721

# STREAM GAS-4

SUBSTREAM MIXED TEMP=1472.84775 PRES=336.63

MOLE-FLOW CO 3369.80386 / H2 5794.40958 / H2O 992.92336

STREAM O2

SUBSTREAM MIXED TEMP=1472.84775 PRES=336.63

MOLE-FLOW O2 4034.62266

STREAM SYNGAS

SUBSTREAM MIXED TEMP=1244.6778 PRES=336.63

MOLE-FLOW CO2 436.365184 / CO 2933.43868 / H2 6230.77476 / &  
H2O 556.558176

DEF-STREAMS HEAT E-1

STREAM E-1

INFO HEAT DUTY=5932.4764 TEMP=1472.3091 TEND=1244.6778

DEF-STREAMS HEAT E-2

STREAM E-2

INFO HEAT DUTY=-265840.498 TEMP=1469.97076 TEND=1472

DEF-STREAMS HEAT E-3

STREAM E-3

INFO HEAT DUTY=-0.06517767

DEF-STREAMS HEAT E-4

STREAM E-4

INFO HEAT DUTY=7197.25105

DEF-STREAMS HEAT ELCPWR

STREAM ELCPWR

INFO HEAT DUTY=-252710.835

DEF-STREAMS HEAT QPROC

STREAM QPROC

INFO HEAT DUTY=0

BLOCK AIR-MIX MIXER

BLOCK Q-MIX MIXER

BLOCK ELDRDS SEP

```

PARAM PRES=336.63
FRAC STREAM=O2 SUBSTREAM=MIXED COMPS=O2 FRACS=1.

BLOCK AIR-TEMP HEATER
PARAM TEMP=1244.67416 PRES=336.63

BLOCK ISOTELC RSTOIC
PARAM TEMP=1472. PRES=3.5 <MPa>
STOIC 1 MIXED H2O -1. / H2 1. / O2 0.5
STOIC 2 MIXED CO2 -1. / CO 1. / O2 0.5
CONV 1 MIXED H2O 0.8361
CONV 2 MIXED CO2 1.

BLOCK GSR-1 RGIBBS
PARAM PRES=0. DUTY=0. <Btu/hr>
PROD H2O / H2 / CO2 / CO
PROD-FRAC N2 1. / O2 1.

BLOCK GSR-2 RGIBBS
PARAM TEMP=1472. PRES=0.
PROD H2O / H2 / CO2 / CO
PROD-FRAC O2 1. / N2 1.

DESIGN-SPEC Q-PROC
F  DOUBLE PRECISION A(5),ASRI(51)
F  COMMON O2LBML
  DEFINE TINF STREAM-VAR STREAM=GAS-2 SUBSTREAM=MIXED &
    VARIABLE=TEMP
  DEFINE TOUTF STREAM-VAR STREAM=SYNGAS SUBSTREAM=MIXED &
    VARIABLE=TEMP
  DEFINE YIH2O MOLE-FRAC STREAM=GAS-2 SUBSTREAM=MIXED &
    COMPONENT=H2O
  DEFINE YOH2O MOLE-FRAC STREAM=SYNGAS SUBSTREAM=MIXED &
    COMPONENT=H2O
  DEFINE YIH2 MOLE-FRAC STREAM=GAS-2 SUBSTREAM=MIXED &
    COMPONENT=H2
  DEFINE YOH2 MOLE-FRAC STREAM=SYNGAS SUBSTREAM=MIXED &
    COMPONENT=H2
  DEFINE YIO2 MOLE-FRAC STREAM=AIR SUBSTREAM=MIXED &
    COMPONENT=O2
  DEFINE YOO2 MOLE-FRAC STREAM=AIR-3 SUBSTREAM=MIXED &
    COMPONENT=O2
  DEFINE PRSPSI STREAM-VAR STREAM=GAS-2 SUBSTREAM=MIXED &
    VARIABLE=PRES
  DEFINE ELECKW INFO-VAR INFO=HEAT VARIABLE=DUTY &
    STREAM=ELCPWR

```

```

C *****
C Aspen Input Variables Needed:
C
C TIN, Temperature In, K
C TOUT, Temperature Out, K
C YIH2O, mole fraction of steam in
C YOH2O, mole fraction of steam out
C YIH2, mole fraction of hydrogen in
C YOH2, mole fraction of hydrogen out
C YIO2, mole fraction of oxygen in
C YOO2, mole fraction of oxygen out
C PRS, Pressure, dBar
C
C *****
C Convert input variables into the appropriate units:
C
F TIN=((TINF-32.)*(5./9.))+273.15
F TOUT=((TOUTF-32.)*(5./9.))+273.15
F PRS=PRSPSI/145.0377
C *****
C Constant Definitions:
C
F A(1)=238241.0
F A(2)=39.9522
F A(3)=3.31866e-003
F A(4)=-3.53216e-008
F A(5)=-12.8498
F FA=96487.0
F RU=8.314
F PAMB=0.101325
C *****
C Inputs:
C NC, number of cells
F NC=3488000.
C AREA, cell area (cm2)
F AREA=225.
C CRTDEN, current density (ampere/cm2)
F CRTDEN=0.25
C ASR, area specific resistance at 1100 K (ohm*cm2)
F ASR=0.2772
C *****
C Calculations:
F CRNT=CRTDEN*AREA
F FLO2=NC*CRNT/(4.0*FA)
F O2LBML=(FLO2/1000.*3600.)*2.2046
C Calculate temp averaged ASR:

```



```

F   DELT=(TOUT-TIN)/50.
F   TEM=TIN
F   ASRI(1)=EXP(10300./TEM)*0.00003973+(ASR-0.463)
F   IF(ABS(TOUT-TIN).LT.0.001) THEN
F     ASRAVE=ASRI(1)
F   ELSE
F     DO 100 I=2,51
F       TEM=TEM+DELT
F       ASRI(I)=EXP(10300./TEM)*0.00003973+(ASR-0.463)
F 100  CONTINUE
F     SUM=ASRI(1)+4.*ASRI(50)+ASRI(51)
F     DO 110 I=1,24
F       SUM=SUM+4.*ASRI(2*I)+2.*ASRI(2*I+1)
F 110  CONTINUE
F     ASRAVE=1./3.*DELT*SUM/(TOUT-TIN)
F   ENDIF
F   DYH2O=YOH2O-YIH2O
F   DYH2=YOH2-YIH2
F   DYO2=YOO2-YIO2
F   SH2O=(YOH2O*DLOG(YOH2O)-YOH2O)-(YIH2O*DLOG(YIH2O)-YIH2O)
F   SH2=(YOH2*DLOG(YOH2)-YOH2)-(YIH2*DLOG(YIH2)-YIH2)
F   SO2=(YOO2*DLOG(YOO2)-YOO2)-(YIO2*DLOG(YIO2)-YIO2)
F   IF(ABS(TOUT-TIN).LT.0.001) THEN
F     C=1./(2.*FA*DYO2*DYH2)
F     TAVE=(TIN+TOUT)/2.
F     DELG=A(5)*TAVE*DLOG(TAVE)
F     DO 200 I=1,4
F       RI=DFLOAT(I)
F       DELG=DELG+A(I)*TAVE**(RI-1.)
F 200  CONTINUE
F     VN=DYH2/2.*DYO2*DLOG(PRS/PAMB)+(SH2O+SH2)*DYO2+SO2/2.*
F $   DYH2
F     VN=C*(DELG*DYH2*DYO2+RU*TAVE*VN)
F   ELSE
F     C=1./(2.*FA*DYO2*DYH2*(TOUT-TIN))
F     DELG=A(5)/2.*(TOUT**2.*(DLOG(TOUT)-1./2.)-TIN**2.*
F $   (DLOG(TIN)-1./2.))
F     DO 300 I=1,4
F       RI=DFLOAT(I)
F       DELG=DELG+A(I)/RI*(TOUT**RI-TIN**RI)
F 300  CONTINUE
F     VN=DYH2/2.*DYO2*DLOG(PRS/PAMB)+(SH2O+SH2)*DYO2+SO2/2.*
F $   DYH2
F     VN=C*(DELG*DYH2*DYO2+RU/2.*(TOUT**2.-TIN**2.)*VN)
F   ENDIF
F   VOP=VN+CRTDEN*ASRAVE

```

```

F  ELPWR=-NC*VOP*CRNT/1000.
C *****
C Output statements:
F  WRITE(NTerm,500)NC,AREA,CRTDEN,ASR
F  WRITE(NRPT,500)NC,AREA,CRTDEN,ASR
F  WRITE(NHSTRY,500)NC,AREA,CRTDEN,ASR
F  WRITE(NTerm,510)ELPWR,VN,VOP,FLO2,O2LBML,CRNT
F  WRITE(NRPT,510)ELPWR,VN,VOP,FLO2,O2LBML,CRNT
F  WRITE(NHSTRY,510)ELPWR,VN,VOP,FLO2,O2LBML,CRNT
F 500 FORMAT(/,6X,'INPUT PARAMETERS:',
F  $/,10X,'NUMBER OF CELLS =',19X,I8,
F  $/,10X,'CELL AREA =',27X,F6.1,1X,'CM2',
F  $/,10X,'CURRENT DENSITY =',21X,F6.4,1X,'AMP/CM2',
F  $/,10X,'AREA SPECIFIC RESISTANCE AT 1100 K =',2X,F6.4,1X,
F  '$OHM*CM2')
F 510 FORMAT(/,6X,'OUTPUT PARAMETERS:',
F  $/,10X,'POWER REQUIREMENT =',17X,F8.0,1X,'KW',
F  $/,10X,'NERNST POTENTIAL =',20X,F6.4,1X,'V',
F  $/,10X,'OPERATING VOLTAGE =',19X,F6.4,1X,'V',
F  $/,10X,'OXYGEN GENERATED =',20X,F6.2,1X,'GMOL/S',
F  $/,10X,'OXYGEN GENERATED =',20X,F6.2,1X,'LBMOL/HR',
F  $/,10X,'CURRENT =',29X,F6.2,1X,'AMPS')
    SPEC "ELECKW" TO "ELPWR"
    TOL-SPEC "0.1"
    VARY BLOCK-VAR BLOCK=GSR-2 VARIABLE=TEMP SENTENCE=PARAM
    LIMITS "1100." "2700."

DESIGN-SPEC T-AIR
    DEFINE TAOUT STREAM-VAR STREAM=ENR-AIR SUBSTREAM=MIXED &
        VARIABLE=TEMP
    DEFINE THOUT STREAM-VAR STREAM=SYNGAS SUBSTREAM=MIXED &
        VARIABLE=TEMP
    SPEC "TAOUT" TO "THOUT"
    TOL-SPEC "0.01"
    VARY BLOCK-VAR BLOCK=AIR-TEMP VARIABLE=TEMP
    SENTENCE=PARAM
    LIMITS "1100." "2700."

STREAM-REPOR MOLEFLOW MASSFLOW MOLEFRAC MASSFRAC

ENDHIERARCHY HT-ELECT

BLOCK AIR-COMP MCOMPR
    PARAM NSTAGE=3 TYPE=ISENTROPIC PRES=336.63
    FEEDS AIR 1
    PRODUCTS AIR-2 3

```

```

COMPR-SPECS 1 SPECS-UTL=ELEC-USE / 2 SPECS-UTL=ELEC-USE / &
3 SPECS-UTL=ELEC-USE
COOLER-SPECS 1 TEMP=104. COOLER-UTL=CW / 2 TEMP=104. &
COOLER-UTL=CW / 3 DUTY=0. COOLER-UTL=CW

```

#### BLOCK B3 MCOMPR

```

PARAM NSTAGE=3 TYPE=ISENTROPIC PRES=336.63
FEEDS WATER 1
PRODUCTS WATER-1 3
COMPR-SPECS 1 SPECS-UTL=ELEC-USE / 2 SPECS-UTL=ELEC-USE / &
3 SPECS-UTL=ELEC-USE
COOLER-SPECS 1 TEMP=1000. COOLER-UTL=CW / 2 TEMP=1000. &
COOLER-UTL=CW / 3 DUTY=0. COOLER-UTL=CW
PERFOR-PARAM CALC-SPEED=NO

```

#### BLOCK CO2-COMP MCOMPR

```

PARAM NSTAGE=3 TYPE=ISENTROPIC PRES=336.63
FEEDS CO2 1
PRODUCTS CO2-1 3
COMPR-SPECS 1 SPECS-UTL=ELEC-USE / 2 SPECS-UTL=ELEC-USE / &
3 SPECS-UTL=ELEC-USE
COOLER-SPECS 1 TEMP=1000. COOLER-UTL=CW / 2 TEMP=1000. &
COOLER-UTL=CW / 3 DUTY=0. COOLER-UTL=CW

```

#### DESIGN-SPEC F-AIR

```

DEFINE AIR STREAM-VAR STREAM=AIR SUBSTREAM=MIXED &
VARIABLE=MASS-FLOW
DEFINE O2 STREAM-VAR STREAM="HT-ELECT.O2" SUBSTREAM=MIXED
&
VARIABLE=MASS-FLOW
SPEC "AIR" TO "1.555*O2"
TOL-SPEC "0.1"
VARY STREAM-VAR STREAM=AIR SUBSTREAM=MIXED &
VARIABLE=MASS-FLOW
LIMITS "200000." "15000000000."

```

#### DESIGN-SPEC F-O2

```

F COMMON O2LBML
DEFINE O2FLOW MOLE-FLOW STREAM="HT-ELECT.O2"
SUBSTREAM=MIXED &
COMPONENT=O2
SPEC "O2FLOW" TO "O2LBML"
TOL-SPEC "0.1"
VARY BLOCK-VAR BLOCK=B1 SENTENCE=MASS-FLOW VARIABLE=FLOW
&
ID1=CO2

```

```

LIMITS "10" "400000."

DESIGN-SPEC R-H2-CO
  DEFINE H2 MOLE-FLOW STREAM="HT-ELECT.SYNGAS"
  SUBSTREAM=MIXED &
    COMPONENT=H2
  DEFINE CO MOLE-FLOW STREAM="HT-ELECT.SYNGAS"
  SUBSTREAM=MIXED &
    COMPONENT=CO
  SPEC "H2/CO" TO "2.12"
  TOL-SPEC "0.01"
  VARY BLOCK-VAR BLOCK=B2 SENTENCE=MOLE-FLOW VARIABLE=FLOW
&
  ID1=WATER
  LIMITS "0" "200000000."

DESIGN-SPEC R-RECYCL
  DEFINE H2 MOLE-FLOW STREAM=HTE-FEED SUBSTREAM=MIXED &
    COMPONENT=H2
  DEFINE CO MOLE-FLOW STREAM=HTE-FEED SUBSTREAM=MIXED &
    COMPONENT=CO
  DEFINE TOTAL STREAM-VAR STREAM=HTE-FEED SUBSTREAM=MIXED &
    VARIABLE=MOLE-FLOW
  SPEC "(H2+CO)/TOTAL" TO "0.1"
  TOL-SPEC "0.01"
  VARY BLOCK-VAR BLOCK=SYN-SPLT SENTENCE=FRAC VARIABLE=FRAC
&
  ID1=RECY-GAS
  LIMITS "0.01" "0.5"

DESIGN-SPEC T-INLET
  DEFINE TIN STREAM-VAR STREAM=HTE-FEED SUBSTREAM=MIXED &
    VARIABLE=TEMP
  SPEC "TIN" TO "1472."
  TOL-SPEC "0.5"
  VARY BLOCK-VAR BLOCK=FEED-HTR VARIABLE=TEMP
  SENTENCE=PARAM
  LIMITS "1100." "2800."

EO-CONV-OPTI

STREAM-REPOR MOLEFLOW MASSFLOW MOLEFRAC MASSFRAC

ENDHIERARCHY HTSE

HIERARCHY PCFB

```

DEF-STREAMS CONVEN ALL

SOLVE

PARAM METHOD=SM

RUN-MODE MODE=SIM

FLOWSHEET

BLOCK B14 IN=18 19 OUT=RELEASE

BLOCK B1 IN=11 OUT=1

BLOCK B2 IN=14 1 OUT=2 3

BLOCK B4 IN=4 3 OUT=5

BLOCK B5 IN=5 OUT=6 7

BLOCK B6 IN=COALAIR2 OUT=8

BLOCK B7 IN=10 16 OUT=12

BLOCK B8 IN=12 OUT=13 17

BLOCK B2-COPY IN=15 8 OUT=9 16

BLOCK B3 IN=2 OUT=19 21

BLOCK B9 IN=9 OUT=18 20

PROPERTIES PR-BM FREE-WATER=STEAM-TA SOLU-WATER=3 TRUE-COMPS=YES

PROPERTIES ELECNRTL / IAPWS-95 / IDEAL / PENG-ROB /  
RKS-BM / WILSON

STREAM 1

SUBSTREAM MIXED TEMP=1603.55368 PRES=174.045285

MOLE-FLOW N2 11275.0072 / O2 5014.46439

STREAM 2

SUBSTREAM MIXED TEMP=1561.99999 PRES=174.045285

MOLE-FLOW WATER 1828.45776 / CO2 4300.89343 / CO &  
474.762408 / N2 11308.5521 / H2 171.17609 / CH4 &  
0.00110178027 / O2 9.064694E-013 / CARBON &  
2.034658E-025 / SULFUR 8.516061E-007 / NO2 &  
3.731216E-017 / NO 2.884731E-008 / HCL 2.41124007 / &  
CL2 1.210420E-011 / SO2 0.0438893818 / C2H4 &  
7.358607E-011 / C2H2 1.430613E-011 / C2H6 &  
3.394747E-012 / C3H8 3.664291E-020 / H3N 0.0446206596 / &  
N2O 5.599543E-012 / O2S 0.0438893818 / O3S &  
5.288328E-010 / H2S 34.5690101

STREAM 4

SUBSTREAM MIXED TEMP=17.900000008 <C> PRES=0.10000000029 <MPa> &  
MASS-FLOW=936964.626

MOLE-FRAC WATER 1

STREAM 5

SUBSTREAM MIXED TEMP=643.948926 PRES=2030.52833  
MOLE-FLOW WATER 52009.4401

STREAM 6

SUBSTREAM MIXED TEMP=146.030313 PRES=3.05359928  
MOLE-FLOW WATER 52009.4401

STREAM 8

SUBSTREAM MIXED TEMP=1603.55368 PRES=174.045285  
MOLE-FLOW N2 11275.0072 / O2 5014.46439

STREAM 9

SUBSTREAM MIXED TEMP=1561.99999 PRES=174.045285  
MOLE-FLOW WATER 1828.45776 / CO2 4300.89343 / CO &  
474.762408 / N2 11308.5521 / H2 171.17609 / CH4 &  
0.00110178027 / O2 9.064694E-013 / CARBON &  
2.034658E-025 / SULFUR 8.516061E-007 / NO2 &  
3.731216E-017 / NO 2.884731E-008 / HCL 2.41124007 / &  
CL2 1.210420E-011 / SO2 0.0438893818 / C2H4 &  
7.358607E-011 / C2H2 1.430613E-011 / C2H6 &  
3.394747E-012 / C3H8 3.664291E-020 / H3N 0.0446206596 / &  
N2O 5.599543E-012 / O2S 0.0438893818 / O3S &  
5.288328E-010 / H2S 34.5690101

STREAM 10

SUBSTREAM MIXED TEMP=17.900000008 <C> PRES=0.10000000029 <MPa> &  
MASS-FLOW=936964.626  
MOLE-FRAC WATER 1

STREAM 11

SUBSTREAM MIXED TEMP=493.622545 PRES=16.696  
MOLE-FLOW N2 11275.0072 / O2 5014.46439

STREAM 12

SUBSTREAM MIXED TEMP=643.948926 PRES=2030.52833  
MOLE-FLOW WATER 52009.4401

STREAM 13

SUBSTREAM MIXED TEMP=146.030313 PRES=3.05359928  
MOLE-FLOW WATER 52009.4401

STREAM 14

SUBSTREAM MIXED TEMP=571.999999 PRES=174.045285

MASS-FLOW N2 940.33468 / H2 4103.27861 / O2 14019.5352 / &  
 CARBON 57360.4155 / SULFUR 1111.30462 / CL2 &  
 85.4849709

#### STREAM 15

SUBSTREAM MIXED TEMP=571.999999 PRES=174.045285  
 MASS-FLOW N2 940.33468 / H2 4103.27861 / O2 14019.5352 / &  
 CARBON 57360.4155 / SULFUR 1111.30462 / CL2 &  
 85.4849709

#### STREAM 18

SUBSTREAM MIXED TEMP=1155.80883 PRES=37.8724902  
 MOLE-FLOW WATER 1828.45776 / CO2 4300.89343 / CO &  
 474.762408 / N2 11308.5521 / H2 171.17609 / CH4 &  
 0.00110178027 / O2 9.064694E-013 / CARBON &  
 2.034658E-025 / SULFUR 8.516061E-007 / NO2 &  
 3.731216E-017 / NO 2.884731E-008 / HCL 2.41124007 / &  
 CL2 1.210420E-011 / SO2 0.0438893818 / C2H4 &  
 7.358607E-011 / C2H2 1.430613E-011 / C2H6 &  
 3.394747E-012 / C3H8 3.664291E-020 / H3N 0.0446206596 / &  
 N2O 5.599543E-012 / O2S 0.0438893818 / O3S &  
 5.288328E-010 / H2S 34.5690101

#### STREAM 19

SUBSTREAM MIXED TEMP=1155.80883 PRES=37.8724902  
 MOLE-FLOW WATER 1828.45776 / CO2 4300.89343 / CO &  
 474.762408 / N2 11308.5521 / H2 171.17609 / CH4 &  
 0.00110178027 / O2 9.064694E-013 / CARBON &  
 2.034658E-025 / SULFUR 8.516061E-007 / NO2 &  
 3.731216E-017 / NO 2.884731E-008 / HCL 2.41124007 / &  
 CL2 1.210420E-011 / SO2 0.0438893818 / C2H4 &  
 7.358607E-011 / C2H2 1.430613E-011 / C2H6 &  
 3.394747E-012 / C3H8 3.664291E-020 / H3N 0.0446206596 / &  
 N2O 5.599543E-012 / O2S 0.0438893818 / O3S &  
 5.288328E-010 / H2S 34.5690101

#### STREAM COALAIR2

SUBSTREAM MIXED TEMP=493.622545 PRES=16.696  
 MOLE-FLOW N2 11275.0072 / O2 5014.46439

#### STREAM RELEASE

SUBSTREAM MIXED TEMP=1155.84778 PRES=14.696  
 MOLE-FLOW WATER 3656.91552 / CO2 8601.78686 / CO &  
 949.524817 / N2 22617.1042 / H2 342.352181 / CH4 &  
 0.00220356054 / O2 1.812938E-012 / CARBON &  
 4.069317E-025 / SULFUR 1.703212E-006 / NO2 &

7.462433E-017 / NO 5.769462E-008 / HCL 4.82248014 / &  
 CL2 2.420841E-011 / SO2 0.0877787636 / C2H4 &  
 1.471721E-010 / C2H2 2.861227E-011 / C2H6 &  
 6.789494E-012 / C3H8 7.328582E-020 / H3N 0.0892413192 / &  
 N2O 1.119908E-011 / O2S 0.0877787636 / O3S &  
 1.057665E-009 / H2S 69.1380203

DEF-STREAMS HEAT 3

STREAM 3

INFO HEAT DUTY=332123.667

DEF-STREAMS HEAT 16

STREAM 16

INFO HEAT DUTY=332123.667

DEF-STREAMS WORK 7

STREAM 7

INFO WORK POWER=-107281.767

DEF-STREAMS WORK 17

STREAM 17

INFO WORK POWER=-107281.767

DEF-STREAMS WORK 20

STREAM 20

INFO WORK POWER=-26820.5051

DEF-STREAMS WORK 21

STREAM 21

INFO WORK POWER=-26820.5051

BLOCK B14 MIXER

PARAM PRES=14.696 NPHASE=1 PHASE=V MAXIT=61 &  
 T-EST=1155.84778

BLOCK-OPTION FREE-WATER=NO ENERGY-BAL=YES

BLOCK B4 HEATER

PARAM PRES=140. <bar>

BLOCK B7 HEATER



PARAM PRES=140. <bar>

BLOCK B2 RGIBBS  
 PARAM TEMP=850. <C> PRES=1.2 <MPa> NPSOL=1 MERGE-SOLIDS=YES  
 PROD WATER / CO2 / CO / N2 / H2 / CH4 / O2 / &  
 ARGON / CARBON / SULFUR / NO2 / NO / HCL / CL2 / &  
 SO2 / C2H4 / C2H2 / C2H6 / C3H8 / H3N / N2O / &  
 O2S / O3S / H2S

BLOCK B2-COPY RGIBBS  
 PARAM TEMP=850. <C> PRES=1.2 <MPa> NPSOL=1 MERGE-SOLIDS=YES  
 PROD WATER / CO2 / CO / N2 / H2 / CH4 / O2 / &  
 ARGON / CARBON / SULFUR / NO2 / NO / HCL / CL2 / &  
 SO2 / C2H4 / C2H2 / C2H6 / C3H8 / H3N / N2O / &  
 O2S / O3S / H2S

BLOCK B1 COMPR  
 PARAM TYPE=ISENTROPIC PRES=1.2 <MPa>

BLOCK B3 COMPR  
 PARAM TYPE=ISENTROPIC POWER=20.000047 <MW> MODEL-  
 TYPE=TURBINE

BLOCK B5 COMPR  
 PARAM TYPE=ISENTROPIC POWER=80. <MW> NPHASE=2 SB-MAXIT=35 &  
 MAXIT=45 MODEL-TYPE=TURBINE  
 BLOCK-OPTION FREE-WATER=NO

BLOCK B6 COMPR  
 PARAM TYPE=ISENTROPIC PRES=1.2 <MPa>

BLOCK B8 COMPR  
 PARAM TYPE=ISENTROPIC POWER=80. <MW> NPHASE=2 SB-MAXIT=35 &  
 MAXIT=45 MODEL-TYPE=TURBINE  
 BLOCK-OPTION FREE-WATER=NO

BLOCK B9 COMPR  
 PARAM TYPE=ISENTROPIC POWER=20.000047 <MW> MODEL-  
 TYPE=TURBINE

EO-CONV-OPTI

ENDHIERARCHY PCFB

HIERARCHY SMR

DEF-STREAMS CONVEN ALL

SOLVE

PARAM METHOD=SM  
RUN-MODE MODE=SIM

FLowsheet

BLOCK B1 IN=6 OUT=7 9  
BLOCK B2 IN=2 1 OUT=3  
BLOCK B3 IN=3 OUT=4 8  
BLOCK B4 IN=5 8 OUT=6

PROPERTIES PR-BM FREE-WATER=STEAM-TA SOLU-WATER=3 TRUE-  
COMPS=YES

PROPERTIES ELECNRTL / IAPWS-95 / IDEAL / PENG-ROB /  
RKS-BM / WILSON

STREAM 2

IN-UNITS SI  
SUBSTREAM MIXED TEMP=277.00000014 <C> PRES=15499.999982 <kPa> &  
MASS-FLOW=2777.777801  
MASS-FRAC H2O 1

STREAM 3

SUBSTREAM MIXED TEMP=622.939999 PRES=5679.74238  
MOLE-FLOW H2O 1223751.53

STREAM 4

SUBSTREAM MIXED TEMP=530.6 PRES=901.727283  
MOLE-FLOW H2O 1223751.53

STREAM 5

IN-UNITS SI  
SUBSTREAM MIXED TEMP=25.000000009 <C> PRES=1.0000000027 <atm> &  
MASS-FLOW=161.11111284  
MASS-FRAC H2O 1

STREAM 6

SUBSTREAM MIXED TEMP=1966.87648 PRES=1247.32454  
MOLE-FLOW H2O 70977.589

STREAM 7

SUBSTREAM MIXED TEMP=935.995817 PRES=14.6959488  
MOLE-FLOW H2O 70977.589

DEF-STREAMS HEAT 1

STREAM 1

IN-UNITS SI

INFO HEAT DUTY=800 <MW>

DEF-STREAMS HEAT 8

STREAM 8

INFO HEAT DUTY=772415.288 TEMP=622.939999 TEND=530.6

DEF-STREAMS WORK 9

STREAM 9

INFO WORK POWER=-282979.326

BLOCK B2 HEATER

IN-UNITS SI

PARAM TEMP=328.3 <C>

BLOCK B3 HEATER

IN-UNITS SI

PARAM TEMP=277. <C> VFRAC=0.

BLOCK B4 HEATER

IN-UNITS SI

PARAM PRES=8600. <kPa>

BLOCK B1 COMPR

IN-UNITS SI

PARAM TYPE=ISENTROPIC PRES=1. <atm> NPHASE=2 MAXIT=40 &  
TOL=0.001 MODEL-TYPE=TURBINE

BLOCK-OPTION FREE-WATER=NO

EO-CONV-OPTI

STREAM-REPOR MOLEFLOW

ENDHIERARCHY SMR

BLOCK B3 MULT

PARAM FACTOR=0.292525635

UTILITY CW GENERAL

COST PRICE=0.

PARAM UTILITY-TYPE=WATER PRES=64.69595 PRES-OUT=54.69595 &

TIN=86. TOUT=122. CALOPT=FLASH

UTILITY ELEC-USE GENERAL

COST ELEC-PRICE=0.

PARAM UTILITY-TYPE=ELECTRICITY

UTILITY LPS-GEN GENERAL

COST PRICE=0.

PARAM UTILITY-TYPE=STEAM PRES=60. PRES-OUT=60. TIN=217. &  
VFR-OUT=1. CALOPT=FLASH

DESIGN-SPEC AIRMULT

DEFINE CARBON MOLE-FLOW STREAM="PCFB.14" SUBSTREAM=MIXED &  
COMPONENT=CARBON

DEFINE MULT BLOCK-VAR BLOCK=B3 VARIABLE=FACTOR &  
SENTENCE=PARAM

DEFINE O2INPUT MOLE-FLOW STREAM=COALAIR SUBSTREAM=MIXED &  
COMPONENT=O2

SPEC "O2INPUT" TO "1.05\*CARBON"

TOL-SPEC ".05"

VARY BLOCK-VAR BLOCK=B3 VARIABLE=FACTOR SENTENCE=PARAM  
LIMITS "0" "10"

EO-CONV-OPTI

CONV-OPTIONS

PARAM TOL=0.0001

WEGSTEIN MAXIT=70

SECANT MAXIT=75 BRACKET=YES

TEAR

TEAR "HTSE.HT-ELECT.GAS-4" / ENR-AIR / "HTSE.RECY-GAS"

STREAM-REPOR MOLEFLOW MASSFLOW MOLEFRAC MASSFRAC NOATTR-  
DESC &

NOSUBS-ATTR

PROPERTY-REP PCES NOPARAM-PLUS

;  
;  
;  
;  
;

## **APPENDIX B.**

### **CONSOLIDATED STEADY STATE ASPEN PLUS INPUT**

The following script is the input file that will generate an Aspen Plus model used in this work. This script will generate the steady state model that was simplified and consolidated from the rigorous model that does not include design specifications nor in-line Fortran programming. This model was used as the flow driven input for the Aspen Dynamics model:

```
;
;Input Summary created by Aspen Plus Rel. 25.0 at 11:26:25 Wed Jul 15, 2015
;Directory Filename C:\Users\klbtz3\Desktop\hes model gutted htse.inp
;

DYNAMICS
  DYNAMICS RESULTS=ON

IN-UNITS ENG ENTHALPY-FLO=kW

DEF-STREAMS CONVEN ALL

SIM-OPTIONS MASS-BAL-CHE=YES FLASH-MAXIT=40 BYPASS-PROP=NO &
  FLASH-METHOD=GIBBS OPER-YEAR=365. <day>

DATABANKS 'APV73 PURE25' / 'APV73 AQUEOUS' / 'APV73 SOLIDS' / &
  'APV73 INORGANIC' / 'APV73 COMBUST' / 'APV73 PURE20' / &
  'APV73 ASPENPCD'

PROP-SOURCES 'APV73 PURE25' / 'APV73 AQUEOUS' / 'APV73 SOLIDS' &
  / 'APV73 INORGANIC' / 'APV73 COMBUST' / 'APV73 PURE20' &
  / 'APV73 ASPENPCD'

COMPONENTS
  WATER H2O /
  CO2 CO2 /
  CO CO /
  N2 N2 /
  H2 H2 /
  CH4 CH4 /
  O2 O2 /
  ARGON AR /
  CARBON C /
  SULFUR S /
  NO2 NO2 /
```

NO NO /  
 HCL HCL /  
 CL2 CL2 /  
 SO2 O2S /  
 H2O H2O /  
 AR AR /  
 C2H4 C2H4 /  
 C2H2 C2H2 /  
 C2H6 C2H6 /  
 C3H8 C3H8 /  
 H3N H3N /  
 N2O N2O /  
 O2S O2S /  
 O3S O3S /  
 H2S H2S /  
 NITRO-01 N2 /  
 OXYGE-01 O2

HENRY-COMPS HC-1 CO2

#### FLOWSHEET

HIERARCHY HTSE  
 CONNECT \$C-3 IN=CO2HTSE OUT="HTSE.CO2HTSE"  
 CONNECT \$C-6 IN=NUCSTEAM OUT="HTSE.NUCSTEAM"  
 CONNECT \$C-4 IN="HTSE.ENR-AIR" OUT=ENR-AIR  
 CONNECT \$C-7 IN="HTSE.SYNGAS-2" OUT=SYNGAS  
 CONNECT \$C-9 IN="HTSE.1" OUT=CO2-XTRA  
 HIERARCHY PCFB  
 CONNECT \$C-5 IN="PCFB.RELEASE" OUT=EFFLUENT  
 CONNECT \$C-1 IN="PCFB.PCFBPWR" OUT=PCFBPWR  
 HIERARCHY SMR  
 CONNECT \$C-8 IN="SMR.7" OUT=NUCSTEAM  
 CONNECT \$C-2 IN="SMR.9" OUT=NUCPWR  
 BLOCK CO2SEP IN=EFFLUENT OUT=CO2HTSE RELEASE

#### PROPERTIES PR-BM

PROPERTIES ELECNRTL / IAPWS-95 / IDEAL / PENG-ROB /  
 RKS-BM / WILSON

#### PROP-DATA REVIEW-1

IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr' &  
 HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=C &  
 VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum' &  
 MASS-DENSITY='kg/cum' MOLE-ENTHALP='kcal/mol' &  
 MASS-ENTHALP='kcal/kg' HEAT=Gcal MOLE-CONC='mol/l' &  
 PDROP=bar

```

PROP-LIST API / DGFORM / DGSFRM / DHFORM / DHSFRM / &
  DHVLB / FREEZEPT / HCOM / MUP / MW / OMEGA / PC / &
  RKTZRA / SG / TB / TC / VB / VC / VLSTD / ZC
PVAL H2O 10.0 / -54.6343 / -56.5492 / -57.7949 / &
  -69.9627 / 9.744507 / 0.0 / 0.0 / 1.84972 / &
  18.01528 / 0.344861 / 220.64 / 0.243172 / 1.0 / &
  100.0 / 373.946 / 18.8311 / 55.9472 / 18.0691 / &
  0.229
PROP-LIST DHFORM / FREEZEPT / MW / PC / VC / VLSTD / &
  ZC / RGYR
PVAL CO2 -94.05110000 / -56.57 / 44.0095 / 73.83 / 94 / &
  61.6782 / 0.274 / 1.04000E-10

PROP-DATA CPDIEC-1
IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr' &
  HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=C &
  VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum' &
  MASS-DENSITY='kg/cum' MOLE-ENTHALP='kcal/mol' &
  MASS-ENTHALP='kcal/kg' HEAT=Gcal MOLE-CONC='mol/l' &
  PDROP=bar
PROP-LIST CPDIEC
PVAL H2O 78.24662286 32730.85746 298.15

PROP-DATA DHVLWT-1
IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr' &
  HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=C &
  VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum' &
  MASS-DENSITY='kg/cum' MOLE-ENTHALP='J/kmol' &
  MASS-ENTHALP='kcal/kg' HEAT=Gcal MOLE-CONC='mol/l' &
  PDROP=bar
PROP-LIST DHVLWT
PVAL H2O 40655000 100.00 0.26623503 0.09110321 0.01

PROP-DATA HENRY-1
IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr' &
  HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=Pa TEMPERATURE=K &
  VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum' &
  MASS-DENSITY='kg/cum' MOLE-ENTHALP='kcal/mol' &
  MASS-ENTHALP='kcal/kg' HEAT=Gcal MOLE-CONC='mol/l' &
  PDROP=bar
PROP-LIST HENRY
BPVAL CO2 H2O 170.7126000 -8477.711000 -21.95743000 &
  5.78074800E-3 273.0000000 500.0000000 0.0

PROP-DATA HENRY-1
IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr' &

```



```

HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=C &
VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum' &
MASS-DENSITY='kg/cum' MOLE-ENTHALP='kcal/mol' &
MASS-ENTHALP='kcal/kg' HEAT=Gcal MOLE-CONC='mol/l' &
PDROP=bar
PROP-LIST HENRY
BPVAL CO2 WATER 159.8650745 -8741.550000 -21.66900000 &
1.10259000E-3 -.1500000000 79.85000000 0.0

```

# PROP-DATA NRTL-1

```

IN-UNITS MET VOLUME-FLOW='cum/hr' ENTHALPY-FLO='Gcal/hr' &
HEAT-TRANS-C='kcal/hr-sqm-K' PRESSURE=bar TEMPERATURE=C &
VOLUME=cum DELTA-T=C HEAD=meter MOLE-DENSITY='kmol/cum' &
MASS-DENSITY='kg/cum' MOLE-ENTHALP='kcal/mol' &
MASS-ENTHALP='kcal/kg' HEAT=Gcal MOLE-CONC='mol/l' &
PDROP=bar
PROP-LIST NRTL
BPVAL H2O CO2 10.06400000 -3268.135000 .2000000000 0.0 0.0 &
0.0 0.0 200.0000000
BPVAL CO2 H2O 10.06400000 -3268.135000 .2000000000 0.0 0.0 &
0.0 0.0 200.0000000
BPVAL WATER CO2 10.06400000 -3268.135000 .2000000000 0.0 &
0.0 0.0 0.0 200.0000000
BPVAL CO2 WATER 10.06400000 -3268.135000 .2000000000 0.0 &
0.0 0.0 0.0 200.0000000
BPVAL WATER H3N -.5440720000 1678.469000 .2000000000 0.0 &
0.0 0.0 0.0 200.0000000
BPVAL H3N WATER -.1642422000 -1027.525000 .2000000000 0.0 &
0.0 0.0 0.0 200.0000000
BPVAL WATER H2S -3.674000000 1155.900000 .2000000000 0.0 &
0.0 0.0 0.0 150.0000000
BPVAL H2S WATER -3.674000000 1155.900000 .2000000000 0.0 &
0.0 0.0 0.0 150.0000000
BPVAL H2O H3N -.5440720000 1678.469000 .2000000000 0.0 0.0 &
0.0 0.0 200.0000000
BPVAL H3N H2O -.1642422000 -1027.525000 .2000000000 0.0 &
0.0 0.0 0.0 200.0000000
BPVAL H2O H2S -3.674000000 1155.900000 .2000000000 0.0 0.0 &
0.0 0.0 150.0000000
BPVAL H2S H2O -3.674000000 1155.900000 .2000000000 0.0 0.0 &
0.0 0.0 150.0000000

```

# PROP-DATA RKSKBV-1

```

IN-UNITS SI
PROP-LIST RKSKBV
BPVAL WATER CO2 .0737000000 0.0 0.0 0.0 1000.000000

```

BPVAL CO2 WATER .0737000000 0.0 0.0 0.0 1000.000000  
 BPVAL CO2 N2 -.0315000000 0.0 0.0 0.0 1000.000000  
 BPVAL N2 CO2 -.0315000000 0.0 0.0 0.0 1000.000000  
 BPVAL CO2 H2 -.3426000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2 CO2 -.3426000000 0.0 0.0 0.0 1000.000000  
 BPVAL CO2 CH4 .0933000000 0.0 0.0 0.0 1000.000000  
 BPVAL CH4 CO2 .0933000000 0.0 0.0 0.0 1000.000000  
 BPVAL CO N2 .0374000000 0.0 0.0 0.0 1000.000000  
 BPVAL N2 CO .0374000000 0.0 0.0 0.0 1000.000000  
 BPVAL CO H2 .0804000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2 CO .0804000000 0.0 0.0 0.0 1000.000000  
 BPVAL CO CH4 .0322000000 0.0 0.0 0.0 1000.000000  
 BPVAL CH4 CO .0322000000 0.0 0.0 0.0 1000.000000  
 BPVAL N2 H2 .0978000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2 N2 .0978000000 0.0 0.0 0.0 1000.000000  
 BPVAL N2 CH4 .0278000000 0.0 0.0 0.0 1000.000000  
 BPVAL CH4 N2 .0278000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2 CH4 -.0222000000 0.0 0.0 0.0 1000.000000  
 BPVAL CH4 H2 -.0222000000 0.0 0.0 0.0 1000.000000  
 BPVAL N2 O2 -7.8000000E-3 0.0 0.0 0.0 1000.000000  
 BPVAL O2 N2 -7.8000000E-3 0.0 0.0 0.0 1000.000000  
 BPVAL N2 ARGON 0.0 0.0 0.0 0.0 1000.000000  
 BPVAL ARGON N2 0.0 0.0 0.0 0.0 1000.000000  
 BPVAL CH4 ARGON .0252000000 0.0 0.0 0.0 1000.000000  
 BPVAL ARGON CH4 .0252000000 0.0 0.0 0.0 1000.000000  
 BPVAL O2 ARGON .0178000000 0.0 0.0 0.0 1000.000000  
 BPVAL ARGON O2 .0178000000 0.0 0.0 0.0 1000.000000  
 BPVAL N2 SO2 .0578000000 0.0 0.0 0.0 1000.000000  
 BPVAL SO2 N2 .0578000000 0.0 0.0 0.0 1000.000000  
 BPVAL CH4 SO2 .1279000000 0.0 0.0 0.0 1000.000000  
 BPVAL SO2 CH4 .1279000000 0.0 0.0 0.0 1000.000000  
 BPVAL CO2 H2O .0737000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2O CO2 .0737000000 0.0 0.0 0.0 1000.000000  
 BPVAL CO2 C2H4 .0533000000 0.0 0.0 0.0 1000.000000  
 BPVAL C2H4 CO2 .0533000000 0.0 0.0 0.0 1000.000000  
 BPVAL N2 AR 0.0 0.0 0.0 0.0 1000.000000  
 BPVAL AR N2 0.0 0.0 0.0 0.0 1000.000000  
 BPVAL N2 C2H4 .0798000000 0.0 0.0 0.0 1000.000000  
 BPVAL C2H4 N2 .0798000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2 C2H4 -.0681000000 0.0 0.0 0.0 1000.000000  
 BPVAL C2H4 H2 -.0681000000 0.0 0.0 0.0 1000.000000  
 BPVAL CH4 AR .0252000000 0.0 0.0 0.0 1000.000000  
 BPVAL AR CH4 .0252000000 0.0 0.0 0.0 1000.000000  
 BPVAL CH4 C2H4 .0189000000 0.0 0.0 0.0 1000.000000  
 BPVAL C2H4 CH4 .0189000000 0.0 0.0 0.0 1000.000000  
 BPVAL O2 AR .0178000000 0.0 0.0 0.0 1000.000000

BPVAL AR O2 .0178000000 0.0 0.0 0.0 1000.000000  
 BPVAL C2H4 C2H2 .0596000000 0.0 0.0 0.0 1000.000000  
 BPVAL C2H2 C2H4 .0596000000 0.0 0.0 0.0 1000.000000  
 BPVAL CO2 C2H6 .1363000000 0.0 0.0 0.0 1000.000000  
 BPVAL C2H6 CO2 .1363000000 0.0 0.0 0.0 1000.000000  
 BPVAL CO C2H6 -.0278000000 0.0 0.0 0.0 1000.000000  
 BPVAL C2H6 CO -.0278000000 0.0 0.0 0.0 1000.000000  
 BPVAL N2 C2H6 .0407000000 0.0 0.0 0.0 1000.000000  
 BPVAL C2H6 N2 .0407000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2 C2H6 -.1667000000 0.0 0.0 0.0 1000.000000  
 BPVAL C2H6 H2 -.1667000000 0.0 0.0 0.0 1000.000000  
 BPVAL CH4 C2H6 -7.8000000E-3 0.0 0.0 0.0 1000.000000  
 BPVAL C2H6 CH4 -7.8000000E-3 0.0 0.0 0.0 1000.000000  
 BPVAL C2H4 C2H6 .0100000000 0.0 0.0 0.0 1000.000000  
 BPVAL C2H6 C2H4 .0100000000 0.0 0.0 0.0 1000.000000  
 BPVAL CO2 C3H8 .1289000000 0.0 0.0 0.0 1000.000000  
 BPVAL C3H8 CO2 .1289000000 0.0 0.0 0.0 1000.000000  
 BPVAL CO C3H8 .0156000000 0.0 0.0 0.0 1000.000000  
 BPVAL C3H8 CO .0156000000 0.0 0.0 0.0 1000.000000  
 BPVAL N2 C3H8 .0763000000 0.0 0.0 0.0 1000.000000  
 BPVAL C3H8 N2 .0763000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2 C3H8 -.2359000000 0.0 0.0 0.0 1000.000000  
 BPVAL C3H8 H2 -.2359000000 0.0 0.0 0.0 1000.000000  
 BPVAL CH4 C3H8 9.00000000E-3 0.0 0.0 0.0 1000.000000  
 BPVAL C3H8 CH4 9.00000000E-3 0.0 0.0 0.0 1000.000000  
 BPVAL C2H6 C3H8 -2.2000000E-3 0.0 0.0 0.0 1000.000000  
 BPVAL C3H8 C2H6 -2.2000000E-3 0.0 0.0 0.0 1000.000000  
 BPVAL WATER H3N -.2800000000 0.0 0.0 0.0 1000.000000  
 BPVAL H3N WATER -.2800000000 0.0 0.0 0.0 1000.000000  
 BPVAL N2 H3N .2222000000 0.0 0.0 0.0 1000.000000  
 BPVAL H3N N2 .2222000000 0.0 0.0 0.0 1000.000000  
 BPVAL ARGON H3N -.2200000000 0.0 0.0 0.0 1000.000000  
 BPVAL H3N ARGON -.2200000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2O H3N -.2800000000 0.0 0.0 0.0 1000.000000  
 BPVAL H3N H2O -.2800000000 0.0 0.0 0.0 1000.000000  
 BPVAL AR H3N -.2200000000 0.0 0.0 0.0 1000.000000  
 BPVAL H3N AR -.2200000000 0.0 0.0 0.0 1000.000000  
 BPVAL CO2 N2O 2.20000000E-3 0.0 0.0 0.0 1000.000000  
 BPVAL N2O CO2 2.20000000E-3 0.0 0.0 0.0 1000.000000  
 BPVAL N2 N2O -.0110000000 0.0 0.0 0.0 1000.000000  
 BPVAL N2O N2 -.0110000000 0.0 0.0 0.0 1000.000000  
 BPVAL CH4 N2O .0211000000 0.0 0.0 0.0 1000.000000  
 BPVAL N2O CH4 .0211000000 0.0 0.0 0.0 1000.000000  
 BPVAL O2 N2O .0433000000 0.0 0.0 0.0 1000.000000  
 BPVAL N2O O2 .0433000000 0.0 0.0 0.0 1000.000000  
 BPVAL N2 O2S .0578000000 0.0 0.0 0.0 1000.000000

BPVAL O2S N2 .0578000000 0.0 0.0 0.0 1000.000000  
 BPVAL CH4 O2S .1279000000 0.0 0.0 0.0 1000.000000  
 BPVAL O2S CH4 .1279000000 0.0 0.0 0.0 1000.000000  
 BPVAL WATER H2S .0100000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2S WATER .0100000000 0.0 0.0 0.0 1000.000000  
 BPVAL CO2 H2S .0989000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2S CO2 .0989000000 0.0 0.0 0.0 1000.000000  
 BPVAL CO H2S .0367000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2S CO .0367000000 0.0 0.0 0.0 1000.000000  
 BPVAL N2 H2S .1696000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2S N2 .1696000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2O H2S .0100000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2S H2O .0100000000 0.0 0.0 0.0 1000.000000  
 BPVAL C2H6 H2S .0852000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2S C2H6 .0852000000 0.0 0.0 0.0 1000.000000  
 BPVAL C3H8 H2S .0885000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2S C3H8 .0885000000 0.0 0.0 0.0 1000.000000  
 BPVAL CO2 NITRO-01 -.0315000000 0.0 0.0 0.0 1000.000000  
 BPVAL NITRO-01 CO2 -.0315000000 0.0 0.0 0.0 1000.000000  
 BPVAL CO NITRO-01 .0374000000 0.0 0.0 0.0 1000.000000  
 BPVAL NITRO-01 CO .0374000000 0.0 0.0 0.0 1000.000000  
 BPVAL N2 OXYGE-01 -7.8000000E-3 0.0 0.0 0.0 1000.000000  
 BPVAL OXYGE-01 N2 -7.8000000E-3 0.0 0.0 0.0 1000.000000  
 BPVAL H2 NITRO-01 .0978000000 0.0 0.0 0.0 1000.000000  
 BPVAL NITRO-01 H2 .0978000000 0.0 0.0 0.0 1000.000000  
 BPVAL CH4 NITRO-01 .0278000000 0.0 0.0 0.0 1000.000000  
 BPVAL NITRO-01 CH4 .0278000000 0.0 0.0 0.0 1000.000000  
 BPVAL O2 NITRO-01 -7.8000000E-3 0.0 0.0 0.0 1000.000000  
 BPVAL NITRO-01 O2 -7.8000000E-3 0.0 0.0 0.0 1000.000000  
 BPVAL ARGON NITRO-01 0.0 0.0 0.0 0.0 1000.000000  
 BPVAL NITRO-01 ARGON 0.0 0.0 0.0 0.0 1000.000000  
 BPVAL ARGON OXYGE-01 .0178000000 0.0 0.0 0.0 1000.000000  
 BPVAL OXYGE-01 ARGON .0178000000 0.0 0.0 0.0 1000.000000  
 BPVAL SO2 NITRO-01 .0578000000 0.0 0.0 0.0 1000.000000  
 BPVAL NITRO-01 SO2 .0578000000 0.0 0.0 0.0 1000.000000  
 BPVAL AR NITRO-01 0.0 0.0 0.0 0.0 1000.000000  
 BPVAL NITRO-01 AR 0.0 0.0 0.0 0.0 1000.000000  
 BPVAL AR OXYGE-01 .0178000000 0.0 0.0 0.0 1000.000000  
 BPVAL OXYGE-01 AR .0178000000 0.0 0.0 0.0 1000.000000  
 BPVAL C2H4 NITRO-01 .0798000000 0.0 0.0 0.0 1000.000000  
 BPVAL NITRO-01 C2H4 .0798000000 0.0 0.0 0.0 1000.000000  
 BPVAL C2H6 NITRO-01 .0407000000 0.0 0.0 0.0 1000.000000  
 BPVAL NITRO-01 C2H6 .0407000000 0.0 0.0 0.0 1000.000000  
 BPVAL C3H8 NITRO-01 .0763000000 0.0 0.0 0.0 1000.000000  
 BPVAL NITRO-01 C3H8 .0763000000 0.0 0.0 0.0 1000.000000  
 BPVAL H3N NITRO-01 .2222000000 0.0 0.0 0.0 1000.000000

BPVAL NITRO-01 H3N .2222000000 0.0 0.0 0.0 1000.000000  
 BPVAL N2O NITRO-01 -.0110000000 0.0 0.0 0.0 1000.000000  
 BPVAL NITRO-01 N2O -.0110000000 0.0 0.0 0.0 1000.000000  
 BPVAL N2O OXYGE-01 .0433000000 0.0 0.0 0.0 1000.000000  
 BPVAL OXYGE-01 N2O .0433000000 0.0 0.0 0.0 1000.000000  
 BPVAL O2S NITRO-01 .0578000000 0.0 0.0 0.0 1000.000000  
 BPVAL NITRO-01 O2S .0578000000 0.0 0.0 0.0 1000.000000  
 BPVAL H2S NITRO-01 .1696000000 0.0 0.0 0.0 1000.000000  
 BPVAL NITRO-01 H2S .1696000000 0.0 0.0 0.0 1000.000000  
 BPVAL NITRO-01 OXYGE-01 -7.8000000E-3 0.0 0.0 0.0 &  
 1000.000000  
 BPVAL OXYGE-01 NITRO-01 -7.8000000E-3 0.0 0.0 0.0 &  
 1000.000000

#### PROP-DATA WILSON-1

IN-UNITS ENG ENTHALPY-FLO=kW

PROP-LIST WILSON

BPVAL WATER H3N -7.914400000 4772.888962 0.0 0.0 &  
 50.00000360 196.7000024 0.0  
 BPVAL H3N WATER 5.290700000 -2178.199963 0.0 0.0 &  
 50.00000360 196.7000024 0.0  
 BPVAL H2O H3N -7.914400000 4772.888962 0.0 0.0 50.00000360 &  
 196.7000024 0.0  
 BPVAL H3N H2O 5.290700000 -2178.199963 0.0 0.0 50.00000360 &  
 196.7000024 0.0

#### STREAM CO2-XTRA

SUBSTREAM MIXED TEMP=1356.69202 PRES=14.696  
 MOLE-FLOW CO2 4786.60317

#### STREAM CO2HTSE

SUBSTREAM MIXED TEMP=1356.69202 PRES=14.696  
 MOLE-FLOW CO2 7753.77273

#### STREAM EFFLUENT

SUBSTREAM MIXED TEMP=1356.69202 PRES=14.696  
 MOLE-FLOW WATER 3651.29426 / CO2 8615.30304 / CO &  
 928.360736 / N2 37791.4222 / H2 322.43285 / CH4 &  
 7.64986955 / O2 2.857755E-014 / CARBON 6.930777E-025 / &  
 SULFUR 2.845282E-008 / NO2 1.186816E-017 / NO &  
 9.666762E-009 / HCL 4.82248014 / CL2 2.586975E-011 / &  
 SO2 0.00142049506 / C2H4 3.173626E-005 / C2H2 &  
 1.050572E-007 / C2H6 8.550991E-005 / C3H8 &  
 3.269350E-009 / H3N 6.80405143 / N2O 1.907675E-011 / &  
 O2S 0.00142049506 / O3S 1.706463E-011 / H2S &  
 69.3107385

## STREAM ENR-AIR

SUBSTREAM MIXED TEMP=1471.99998 PRES=336.63  
 MASS-FLOW N2 153995.974 / O2 46759.3213

## STREAM NUCSTEAM

SUBSTREAM MIXED TEMP=935.995817 PRES=14.6959488  
 MOLE-FLOW H2O 70977.589

## STREAM RELEASE

SUBSTREAM MIXED TEMP=1356.69202 PRES=14.696  
 MOLE-FLOW WATER 3651.29426 / CO2 861.530304 / CO &  
 928.360736 / N2 37791.4222 / H2 322.43285 / CH4 &  
 7.64986955 / SULFUR 2.845282E-008 / NO 9.666762E-009 / &  
 HCL 4.82248014 / CL2 2.586975E-011 / SO2 &  
 0.00142049506 / C2H4 3.173626E-005 / C2H2 &  
 1.050572E-007 / C2H6 8.550991E-005 / C3H8 &  
 3.269350E-009 / H3N 6.80405143 / N2O 1.907675E-011 / &  
 O2S 0.00142049506 / O3S 1.706463E-011 / H2S &  
 69.3107385

## STREAM SYNGAS

SUBSTREAM MIXED TEMP=1472 PRES=336.63  
 MOLE-FLOW CO 2581.43752 / H2 5443.76406

## DEF-STREAMS WORK NUCPWR

## DEF-STREAMS WORK PCFBPWR

## BLOCK CO2SEP SEP

FRAC STREAM=CO2HTSE SUBSTREAM=MIXED COMPS=WATER CO2 CO &  
 N2 H2 CH4 O2 ARGON CARBON SULFUR NO2 NO HCL CL2 &  
 SO2 H2O AR C2H4 C2H2 C2H6 C3H8 H3N N2O O2S O3S H2S &  
 NITRO-01 OXYGE-01 FRACS=0. 0.9 0. 0. 0. 0. 0. 0. &  
 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. &  
 0. 0. 0. 0. 0.

## HIERARCHY HTSE

## DEF-STREAMS CONVEN ALL

## SOLVE

PARAM METHOD=SM  
 RUN-MODE MODE=SIM

# FLOWSHEET

BLOCK AIR-HTR IN=AIR-2 OUT=HOT-AIR  
 BLOCK FEED-HTR IN=WATER-1 CO2-1 OUT=HTE-FEED  
 BLOCK CO2-COMP IN=CO2 OUT=CO2-1  
 BLOCK AIR-COMP IN=AIR OUT=AIR-2  
 BLOCK B1 IN=CO2HTSE OUT=CO2 1  
 BLOCK B2 IN=NUCSTEAM OUT=XTRASTM WATER  
 BLOCK B3 IN=WATER OUT=WATER-1  
 BLOCK HTSE IN=HTE-FEED OUT=3  
 BLOCK B7 IN=3 OUT=SYNGAS-2 4 5  
 BLOCK B8 IN=HOT-AIR 5 OUT=ENR-AIR  
 BLOCK B9 IN=PWR-REQD HT-INPUT OUT=6

## PROPERTIES PR-BM

PROPERTIES ELECNRTL / IAPWS-95 / IDEAL / PENG-ROB /  
 RKS-BM / WILSON

## STREAM 1

SUBSTREAM MIXED TEMP=1356.69202 PRES=14.696  
 MOLE-FLOW CO2 4786.60317

## STREAM AIR

SUBSTREAM MIXED TEMP=77 PRES=1.0000000027 <atm> &  
 MASS-FLOW=200755.295  
 MOLE-FRAC N2 0.79 / O2 0.21

## STREAM AIR-2

SUBSTREAM MIXED TEMP=372.762308 PRES=336.63  
 MOLE-FLOW N2 5497.20969 / O2 1461.28359

## STREAM CO2

SUBSTREAM MIXED TEMP=1356.69202 PRES=14.696  
 MOLE-FLOW CO2 2967.16957

## STREAM CO2-1

SUBSTREAM MIXED TEMP=1362.30173 PRES=336.63  
 MOLE-FLOW CO2 2967.16957

## STREAM CO2HTSE

SUBSTREAM MIXED TEMP=1356.69202 PRES=14.696  
 MOLE-FLOW CO2 7753.77273

## STREAM ENR-AIR

SUBSTREAM MIXED TEMP=1471.99998 PRES=336.63  
 MOLE-FLOW N2 5497.20969 / O2 1461.28359

STREAM HOT-AIR

SUBSTREAM MIXED TEMP=1472 PRES=336.63

MOLE-FLOW N2 5497.20969 / O2 1461.28359

STREAM HTE-FEED

SUBSTREAM MIXED TEMP=1472 PRES=336.63

MOLE-FLOW CO2 2967.16957 / H2O 5976.362

STREAM NUCSTEAM

SUBSTREAM MIXED TEMP=935.995817 PRES=14.6959488

MOLE-FLOW H2O 70977.589

STREAM SYNGAS-2

SUBSTREAM MIXED TEMP=1472 PRES=336.63

MOLE-FLOW CO 2581.43752 / H2 5443.76406

STREAM WATER

SUBSTREAM MIXED TEMP=935.995817 PRES=1.0000000027 <atm>

MOLE-FLOW H2O 5976.362

STREAM WATER-1

SUBSTREAM MIXED TEMP=1486.31538 PRES=336.63

MOLE-FLOW H2O 5976.362

STREAM XTRASTM

SUBSTREAM MIXED TEMP=935.995817 PRES=14.6959488

MOLE-FLOW H2O 65001.227

DEF-STREAMS HEAT 6

DEF-STREAMS HEAT HT-INPUT

STREAM HT-INPUT

INFO HEAT DUTY=0

DEF-STREAMS HEAT PWR-REQD

STREAM PWR-REQD

INFO HEAT DUTY=-252710.835

BLOCK B8 MIXER

BLOCK B9 MIXER

BLOCK B1 FSPLIT

MASS-FLOW CO2 130583.649



## BLOCK B2 FSPLIT

MOLE-FLOW WATER 5976.362

## BLOCK B7 SEP

FRAC STREAM=SYNGAS-2 SUBSTREAM=MIXED COMPS=WATER CO2 CO  
&

N2 H2 CH4 O2 ARGON CARBON SULFUR NO2 NO HCL CL2 &  
SO2 H2O AR C2H4 C2H2 C2H6 C3H8 H3N N2O O2S O3S H2S &  
NITRO-01 OXYGE-01 FRACS=0. 0. 1. 0. 1. 0. 0. 0. 0. &  
0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. &  
0. 0. 0. 0.

FRAC STREAM=5 SUBSTREAM=MIXED COMPS=WATER CO2 CO N2 H2 &  
CH4 O2 ARGON CARBON SULFUR NO2 NO HCL CL2 SO2 H2O &  
AR C2H4 C2H2 C2H6 C3H8 H3N N2O O2S O3S H2S NITRO-01 &  
OXYGE-01 FRACS=0. 0. 0. 1. 0. 0. 1. 0. 0. 0. 0. &  
0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. 0. &  
0. 0.

## BLOCK AIR-HTR HEATER

PARAM TEMP=1472. PRES=0. NPHASE=1 PHASE=V  
BLOCK-OPTION FREE-WATER=NO

## BLOCK FEED-HTR HEATER

PARAM TEMP=1472 PRES=0. NPHASE=1 PHASE=V  
BLOCK-OPTION FREE-WATER=NO

## BLOCK HTSE RSTOIC

PARAM TEMP=1472. PRES=336.63 NPHASE=1 PHASE=V  
STOIC 1 MIXED CO2 -1. / H2O -2. / H2 2. / CO 1. / &  
O2 1.5  
STOIC 2 MIXED H2O -2. / H2 2. / O2 1.  
CONV 1 MIXED CO2 0.87  
CONV 2 MIXED H2O 0.047  
BLOCK-OPTION FREE-WATER=NO

## BLOCK AIR-COMP MCOMPR

PARAM NSTAGE=3 TYPE=ISENTROPIC PRES=336.63  
FEEDS AIR 1  
PRODUCTS AIR-2 3  
COMPR-SPECS 1 SPECS-UTL=ELEC-USE / 2 SPECS-UTL=ELEC-USE / &  
3 SPECS-UTL=ELEC-USE  
COOLER-SPECS 1 TEMP=104. COOLER-UTL=CW / 2 TEMP=104. &  
COOLER-UTL=CW / 3 DUTY=0. COOLER-UTL=CW

## BLOCK B3 MCOMPR

```

PARAM NSTAGE=3 TYPE=ISENTROPIC PRES=336.63
FEEDS WATER 1
PRODUCTS WATER-1 3
COMPR-SPECS 1 SPECS-UTL=ELEC-USE / 2 SPECS-UTL=ELEC-USE / &
  3 SPECS-UTL=ELEC-USE
COOLER-SPECS 1 TEMP=1000. COOLER-UTL=CW / 2 TEMP=1000. &
  COOLER-UTL=CW / 3 DUTY=0. COOLER-UTL=CW
PERFOR-PARAM CALC-SPEED=NO

BLOCK CO2-COMP MCOMPR
PARAM NSTAGE=3 TYPE=ISENTROPIC PRES=336.63
FEEDS CO2 1
PRODUCTS CO2-1 3
COMPR-SPECS 1 SPECS-UTL=ELEC-USE / 2 SPECS-UTL=ELEC-USE / &
  3 SPECS-UTL=ELEC-USE
COOLER-SPECS 1 TEMP=1000. COOLER-UTL=CW / 2 TEMP=1000. &
  COOLER-UTL=CW / 3 DUTY=0. COOLER-UTL=CW

EO-CONV-OPTI

STREAM-REPOR MOLEFLOW MASSFLOW MOLEFRAC MASSFRAC

ENDHIERARCHY HTSE

HIERARCHY PCFB

DEF-STREAMS CONVEN ALL

SOLVE
PARAM METHOD=SM
RUN-MODE MODE=SIM

FLOWSHEET
BLOCK B14 IN=PCFB1 PCFB2 OUT=RELEASE
BLOCK B1 IN=EFFTURB2 STMTURB2 OUT=3
BLOCK B2 IN=STMTURB1 EFFTURB1 OUT=1
BLOCK B3 IN=1 3 OUT=PCFBPWR

PROPERTIES PR-BM FREE-WATER=STEAM-TA SOLU-WATER=3 TRUE-
COMPS=YES
PROPERTIES ELECNRTL / IAPWS-95 / IDEAL / PENG-ROB /
RKS-BM / WILSON

STREAM PCFB1
SUBSTREAM MIXED TEMP=1561.99999 PRES=174.045285

```

MOLE-FLOW WATER 1825.64713 / CO2 4307.65152 / CO &  
 464.180368 / N2 18895.7111 / H2 161.216425 / CH4 &  
 3.82493477 / O2 1.428877E-014 / CARBON 3.465388E-025 / &  
 SULFUR 1.422641E-008 / NO2 5.934084E-018 / NO &  
 4.833381E-009 / HCL 2.41124007 / CL2 1.293487E-011 / &  
 SO2 0.00071024752 / C2H4 1.586813E-005 / C2H2 &  
 5.252861E-008 / C2H6 4.275495E-005 / C3H8 &  
 1.634675E-009 / H3N 3.40202572 / N2O 9.538375E-012 / &  
 O2S 0.00071024752 / O3S 8.532318E-012 / H2S &  
 34.6553692

#### STREAM PCFB2

SUBSTREAM MIXED TEMP=1561.99999 PRES=174.045285  
 MOLE-FLOW WATER 1825.64713 / CO2 4307.65152 / CO &  
 464.180368 / N2 18895.7111 / H2 161.216425 / CH4 &  
 3.82493477 / O2 1.428877E-014 / CARBON 3.465388E-025 / &  
 SULFUR 1.422641E-008 / NO2 5.934084E-018 / NO &  
 4.833381E-009 / HCL 2.41124007 / CL2 1.293487E-011 / &  
 SO2 0.00071024752 / C2H4 1.586813E-005 / C2H2 &  
 5.252861E-008 / C2H6 4.275495E-005 / C3H8 &  
 1.634675E-009 / H3N 3.40202572 / N2O 9.538375E-012 / &  
 O2S 0.00071024752 / O3S 8.532318E-012 / H2S &  
 34.6553692

#### STREAM RELEASE

SUBSTREAM MIXED TEMP=1356.69202 PRES=14.696  
 MOLE-FLOW WATER 3651.29426 / CO2 8615.30304 / CO &  
 928.360736 / N2 37791.4222 / H2 322.43285 / CH4 &  
 7.64986955 / O2 2.857755E-014 / CARBON 6.930777E-025 / &  
 SULFUR 2.845282E-008 / NO2 1.186816E-017 / NO &  
 9.666762E-009 / HCL 4.82248014 / CL2 2.586975E-011 / &  
 SO2 0.00142049506 / C2H4 3.173626E-005 / C2H2 &  
 1.050572E-007 / C2H6 8.550991E-005 / C3H8 &  
 3.269350E-009 / H3N 6.80405143 / N2O 1.907675E-011 / &  
 O2S 0.00142049506 / O3S 1.706463E-011 / H2S &  
 69.3107385

DEF-STREAMS WORK 1

DEF-STREAMS WORK 3

DEF-STREAMS WORK EFFTURB1

STREAM EFFTURB1

INFO WORK POWER=-26820.499

DEF-STREAMS WORK EFFTURB2

STREAM EFFTURB2

INFO WORK POWER=-26820.4988

DEF-STREAMS WORK PCFBPWR

DEF-STREAMS WORK STMTURB1

STREAM STMTURB1

INFO WORK POWER=-107281.77

DEF-STREAMS WORK STMTURB2

STREAM STMTURB2

INFO WORK POWER=-107281.767

BLOCK B1 MIXER

BLOCK B2 MIXER

BLOCK B3 MIXER

BLOCK B14 MIXER

PARAM PRES=14.696 NPHASE=1 PHASE=V MAXIT=61 &  
T-EST=1356.69202

BLOCK-OPTION FREE-WATER=NO ENERGY-BAL=YES

EO-CONV-OPTI

ENDHIERARCHY PCFB

HIERARCHY SMR

DEF-STREAMS CONVEN ALL

SOLVE

PARAM METHOD=SM

RUN-MODE MODE=SIM

FLOWSHEET

BLOCK B1 IN=6 OUT=7 9

BLOCK B2 IN=2 1 OUT=3

BLOCK B3 IN=3 OUT=4 8

BLOCK B4 IN=5 8 OUT=6

PROPERTIES PR-BM FREE-WATER=STEAM-TA SOLU-WATER=3 TRUE-  
COMPS=YES

PROPERTIES ELECNRTL / IAPWS-95 / IDEAL / PENG-ROB /  
RKS-BM / WILSON

STREAM 2

IN-UNITS SI

SUBSTREAM MIXED TEMP=277.00000014 <C> PRES=15499.999982 <kPa> &

MASS-FLOW=2777.777801

MASS-FRAC H2O 1

STREAM 3

SUBSTREAM MIXED TEMP=622.939999 PRES=5679.74238

MOLE-FLOW H2O 1223751.53

STREAM 4

SUBSTREAM MIXED TEMP=530.6 PRES=901.727283

MOLE-FLOW H2O 1223751.53

STREAM 5

IN-UNITS SI

SUBSTREAM MIXED TEMP=25.000000009 <C> PRES=1.0000000027 <atm> &

MASS-FLOW=161.11111284

MASS-FRAC H2O 1

STREAM 6

SUBSTREAM MIXED TEMP=1966.87648 PRES=1247.32454

MOLE-FLOW H2O 70977.589

STREAM 7

SUBSTREAM MIXED TEMP=935.995817 PRES=14.6959488

MOLE-FLOW H2O 70977.589

DEF-STREAMS HEAT 1

STREAM 1

IN-UNITS SI

INFO HEAT DUTY=800 <MW>

DEF-STREAMS HEAT 8

STREAM 8

INFO HEAT DUTY=772415.288 TEMP=622.939999 TEND=530.6

DEF-STREAMS WORK 9

STREAM 9

INFO WORK POWER=-282979.326

BLOCK B2 HEATER

IN-UNITS SI

PARAM TEMP=328.3 <C>

BLOCK B3 HEATER

IN-UNITS SI

PARAM TEMP=277. <C> VFRAC=0.

BLOCK B4 HEATER

IN-UNITS SI

PARAM PRES=8600. <kPa>

BLOCK B1 COMPR

IN-UNITS SI

PARAM TYPE=ISENTROPIC PRES=1. <atm> NPHASE=2 MAXIT=40 &

TOL=0.001 MODEL-TYPE=TURBINE

BLOCK-OPTION FREE-WATER=NO

EO-CONV-OPTI

STREAM-REPOR MOLEFLOW

ENDHIERARCHY SMR

UTILITY CW GENERAL

COST PRICE=0.

PARAM UTILITY-TYPE=WATER PRES=64.69595 PRES-OUT=54.69595 &

TIN=86. TOUT=122. CALOPT=FLASH

UTILITY ELEC-USE GENERAL

COST ELEC-PRICE=0.

PARAM UTILITY-TYPE=ELECTRICITY

UTILITY LPS-GEN GENERAL

COST PRICE=0.

PARAM UTILITY-TYPE=STEAM PRES=60. PRES-OUT=60. TIN=217. &

VFR-OUT=1. CALOPT=FLASH

EO-CONV-OPTI

CONV-OPTIONS

PARAM TOL=0.0001

WEGSTEIN MAXIT=70  
SECANT MAXIT=75 BRACKET=YES

STREAM-REPOR MOLEFLOW MASSFLOW MOLEFRAC MASSFRAC NOATTR-  
DESC &  
NOSUBS-ATTR

PROPERTY-REP PCES NOPARAM-PLUS

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## VITA

Kyle Lee Buchheit was born on July 14, 1987. He attended Oak Ridge R-VI High School, where he graduated valedictorian of the class of 2006. It was during his final summer break that he had visited the University of Missouri – Rolla Jackling Intro to Engineering summer camp which defined what university he would attend upon graduation.

He completed his B.S. degree in Chemical Engineering with a B.A. degree in Economics at the Missouri University of Science and Technology in May of 2010. He was approached by a faculty member to join his group of molecular dynamics research. After discovering it wasn't a good fit, he joined Dr. Joseph Smith's research group in the fall of 2011.

During this time he also worked with Dr. John Singler to complete his M.S. degree in Applied Mathematics at the Missouri University of Science and Technology in May of 2013. He was also a Chancellor's Fellowship recipient, GAANN recipient, graduate research assistant, graduate teaching assistant, and course instructor during his time as a graduate student in the Chemical and Biochemical Engineering Department while pursuing his Ph.D. Kyle Buchheit graduated with his Ph.D. in Chemical Engineering in December of 2015.