SUPERSTRUCTURE OPTIMIZATION OF HYDROGEN PRODUCTION FROM BIOMASS VIA GASIFICATION

By

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CERTIFICATION OF APPROVAL

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Approved by,

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CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

(ASMA' BINTI AHMADON)

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First of all, the highest praises are due to gracious of The Almighty Lord for granting strength and allowing the completion of this project despite difficulties encountered.

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ABSTRACT

Hydrogen has special properties to replace fossil fuels as a renewable energy source. It is more energy efficient than gasoline, where it can store approximately 2.6 times more energy per unit mass than gasoline. Sourcing hydrogen from biomass is more environmentally friendly as the sustainability factor is covered. Biomass gasification has a promising future to replace fossil fuels. Its carbon neutral characteristic proves its suitability in today's current ecosystem condition. In this work, a mixed-integer superstructure optimization framework is proposed on the cost minimization problem for determining the optimal feasible route for hydrogen production from biomass through gasification. We are interested to investigate various feasible technologies and methods available with their operating conditions that are linear/equality constraints to the conceptual process synthesis problem of the design of the most cost effective gasification route. Possible processes and technologies discussed in recent literature are compiled into a superstructure model. The superstructure modeling and optimization are solved in MATLAB to identify the most cost effective route.

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INTRODUCTION

1.1 BACKGROUND OF STUDY

1.1.1 Energy Crisis

Crude oil, coal and gas are the main resources for world energy supply. Across the globe, many doubt when non-renewable energy will be diminished. It is expected that the global energy market will continue to depend on fossil fuels for at least the next few decades. The World Energy Outlook (WEO) 2007 claims that the energy generated from fossil fuels will remain the major source and is still expected to meet about 84% of energy demand in 2030 (Shafiee and Topal, 2009).

A research by Moriarty and Honnery (2009) explains on how much energy we will consume annually in the future and what sources of energy we will be using. They argued that no high energy future case is probable, because of resource limitations, and rising energy, environmental and money costs per unit of delivered energy as annual energy demand rises far beyond present levels (Moriarty and Honnery, 2009).

The reserves of oil and gas did not decline over the last few decades, and predictions that oil and gas are diminishing were not reliable (Shafiee and Topal, 2009). However, they did predict that the reserves of non-renewable energy sources will last at the closest of 40 years soon. This is the main reason why this project focuses on improving and meeting the energy demand of the future despite current sources depleting.

1.1.2 Alternative Energy Sources

Research conducted by Shafiee and Topal resulted with coal as the main substitution of energy for oil and gas due to its huge reserve and cheap. On the other hand, clean coal and environmental problems are still barriers for coal expanding as a major fossil fuel. Their paper recommended further research into other variables that influence the fluctuation of fossil fuel reserves, especially technological solutions that may facilitate the consumption of coal as a clean energy (Shafiee and Topal, 2009). Even though coal was suggested as the next possible energy resource, environmental effects may become the major drawbacks to further expand future plans for substituting it for oil and gas.

Thaksale et al (2010) proposed hydrogen as the possible future fuel. The inter-related problems of energy and environment are among the biggest challenges facing the world today, in particular energy sustainability and carbon emissions from the fossil fuels. Hydrogen has been projected as one of the few long-term sustainable clean energy carriers, emitting only water vapour as a by-product during the combustion or oxidation process. However, hydrogen is not readily available in sufficient quantities and the production cost is still high for transportation purpose (Thaksale et al, 2010).Santili agreed with this by adding special properties when hydrogen is used as transportation fuel (Santili, 2003).

To overcome hallenges, possible routes to large-scale introduction of hydrogen can conveniently be reduced to three. First, hydrogen could be introduced because of various technical breakthroughs, either leading to strong direct demand for hydrogen, or to direct production of hydrogen. Second, increasing the share of intermittent renewable energy in electricity grids would eventually require either dumping of electricity if excess to requirements, or else conversion to some other energy form and storage – with hydrogen, a strong contender. Third, conversion of electricity to hydrogen would seem unlikely any time soon. Only after electricity needs were fully met by CO_2 emission-free sources would hydrogen production from any excess electricity generation be considered (Moriarty and Honnery, 2009).

1.1.3 Hydrogen from Biomass

Biomass has the potential to accelerate the realization of hydrogen as a major fuel of the future. Since biomass is renewable and consumes atmospheric CO_2 during growth, it can have a small net CO_2 impact compared to fossil fuels. However, hydrogen from biomass has major challenges.

There are no completed technology demonstrations. The yield of hydrogen is low from biomass since the hydrogen content in biomass is low to begin with (approximately 6% versus 25% for methane) and the energy content is low due to the 40% oxygen content of biomass. The cost for growing, harvesting and transporting biomass is high. Thus, even with reasonable energy efficiencies, it is not presently economically competitive with natural gas steam reforming for stand-alone hydrogen without the advantage of high-value co-products. Additionally, as with all sources of hydrogen, production from biomass will require appropriate hydrogen storage and utilization systems to be developed and deployed (Milne et al., 2001).

From the Malaysian Palm Oil statistics in the year 2009, the development of palm oil production across the years of 2005-2009, it is expected that the palm oil production can be increased to 0.7 million tonnes per year. (Malaysian Palm Oil Statistics 2009, 2010) Malaysian recorded higher export volume, amassing a total of RM 59.77 billion in revenue for 2010. The total palm oil planted area has also increased 3.47 % from 4.69 million ha to 4.85 million ha in 2010. (Annual Report 2010 - Leveraging on Sustainability, 2011)

There are several established and developing technologies to produce hydrogen from various sources. These technologies can be characterized in three categories: (a) net positive emission of CO and CO_2, (b) CO_2 free emissions, and (c) CO_2 natural emissions. Hydrogen production can be environmentally friendly only if the resource used to extract hydrogen is carbon neutral.

CO_2 neutral hydrogen production can be achieved by the conversion of biomass via gasification, pyrolisis of bio-oils, steam reforming of biomass derived higher alkanes and alcohols, and aqueous phase reforming of oxygenated hydrocarbons. Biomass derived hydrogen can be classified as carbon neutral because the CO_2 released during hydrogen production is consumed by further biomass generation (neglecting the CO_2 produced from the fossil fuel energy required for operating the hydrogen production unit) (Tanksale et al., 2010).

The possible processes to convert biomass into hydrogen are gasification, pyrolysis and hydrolysis. Gasification produces gaseous products; pyrolysis produces bio-oils prior to gas and hydrolysis of cellulose to produce sugar monomers.

Syn-gas can be converted to hydrogen by water gas shift (WGS) reaction; however, any remaining CO must be removed from the gas stream. Pyrolysis bio-oil can be converted to liquid fuel but the processes are complex and the conversion is low. Hydrogen can be produced from the bio-oil by autothermal reforming with high conversion efficiency, especially with the use of catalytic membrane reactors. Aqueous phase reforming can be used to convert sugars and sugar alcohols, such as sorbitol, to produce hydrogen. In addition to these, there are other biological (enzymatic and bacterial) routes to produce hydrogen, but the scope of this review is restricted to the heterogeneous catalytic routes only.

Hence based on this variation of possible technologies and operating conditions, an extensive range of investigation is possible. One of the methods to identify the most feasible route is to perform cost minimization via superstructure optimization.

1.1.4 Superstructure Optimization

Process optimization is a major objective in designing a process route. Upon listing possible solutions, the best alternatives are selected to ensure optimal process. This requires analysis of the process with respect to the desired objectives. Different selections of set of processes are possible in order to satisfy the desired objectives.

Due to many possible routes to produce hydrogen from biomass via gasification, a superstructure can be created to represent different possibilities. The superstructure acts as the overriding model, capturing all the possible alternatives and intersections between process components. For each block, several alternative technologies and types of equipment are available for selection.

Several papers have discussed on superstructure optimization involving biomass treatments. Martin and Grossman (2010) analyzed the alternatives of designing bioethanol plants by describing using a superstructure. They optimized using a special decomposition technique, modeled using mixed-integer non-linear programming (MINLP) (Martin & Grossman, 2010). Liu et al. (2009) did a research for polygeneration energy systems design using mixed-integer optimization approach. The superstructure is introduced according to partitions of of major processes. The MINLP model was then developed for design optimization All combinations of technologies and types of equipments form the design space of the plant. The optimal process design will then correspond to the best combination of these components, obtained by eliminating existence of units and links between them. (Liu, Pistikopoulos, & Li, 2009)

1.2 PROBLEM STATEMENT

Possible routes and technologies of hydrogen production are still under study for the optimal hydrogen production process. Biomass is the source of hydrogen production of attractive potential because the thermo-chemical process of biomass offers zero net carbon dioxide. Many processes are available to convert biomass into hydrogen. There are also many variations of operating conditions for optimal production of hydrogen from biomass via gasification leading to the problem of the most optimal production route to solve the energy crisis. Furthermore, each route indicates differing cost factor values which is dependent on the operating conditions; which includes high temperature and pressure, catalyst type and gasification agent used.

1.3. OBJECTIVES AND SCOPE OF STUDY

The expected objectives to be achieved in this work are as follows:

- To identify feasible routes for hydrogen production from biomass via gasification.
- To develop a superstructure model that incorporates the feasible routes of hydrogen production from biomass via gasification with a suitable level of detail and abstraction by considering the processing alternatives of gasification and hydrogen production.
- To formulate an optimization model based on the superstructure model to solve for the optimal production route.

For this project, the work consists of developing a superstructure consisting of linear mathematical models to represent the production routes of hydrogen from biomass via gasification that captures the variations in the operating conditions. The production routes available are extracted from literature review of previous works. The multi-integer linear programming (MILP) superstructure model is then implemented in MATLAB for process simulation. Upon analysis of results, the optimal feasible route is identified as the most cost effective way to produce hydrogen from biomass via gasification.

1.4 RELEVANCY OF PROJECT

The most important of the applicability of a mathematical modeling in real life situation, is its flexibility for use to solve industry-relevant-sized problems. This project is targeted to find out which production route is worth investing by attaining the most feasible route for process design before applying the decision into real life situations.

CHAPTER 2
LITERATURE REVIEW AND THEORY

2.1 Gasification of biomass

The gasification of biomass is a thermal treatment, which results in high production of gaseous products and small quantities of char and ash. It is a well-known technology that can be classified depending on the gasifying agent: air, steam, steam–oxygen, air–steam, oxygen-enriched air, etc. Gasification is carried out at high temperatures in order to optimize the gas production (Balat, Balat, Kirtay, & Balat, 2009).

Irrespective of the reactor configuration, it is believed that gasification occurs in the sequential steps of drying, devolatilization and gasification. There are no sharp boundaries between the steps, and these boundaries often overlap (Kaushal, Abedi, & Mahinpey, 2010).

Koroneos et al. (2008) presented the environmental feasibility and efficiency of producing hydrogen from biomass via two processes. Biomass gasification followed by reforming of the syngas was compared to gasification followed by electricity generation and electrolysis. Biomass-gasification electricity-electrolysis route was found to give better environmental performance than the biomass-gasification-steam reforming-Pressure Swing Absorption (PSA) route. It was assumed that the biomass-gasification-power plant produced all the electricity required for electrolysis and liquefaction steps without need of addition power source. But gasification-electricity-electrolysis route had 92.9% share of renewable energy in the primary energy input.

Fujimoto et al. (2007) gasified woody biomass in steam at high temperature (649.85 ^{o}C) and pressure (6.5 MPa) in the presence of a CO_2 sorbent using a batch reactor with 50 cm^3 capacity. The evolved CO_2 was completely absorbed in the sorbent, and no CO_2 was in the gas phase. Gas conversion ratio was 50% at 649.85 ^{o}C.

Mahishi and Goswami (2007) investigated a novel technique that enhanced the hydrogen yield of conventional biomass steam gasification. This was done by integrating the gasification and absorption reactions. The method involved steam gasification of a carbonaceous fuel (biomass) in presence of a CO_2 sorbent. Experiments were conducted by gasifying pine bark in presence of calcium oxide. The gasification was performed at atmospheric pressure ranging from 500-700 ^oC. The hydrogen yield, total gas yield and carbon conversion efficiency increased by 48.6%, 62.2% and 83.5%, respectively, in the presence of sorbent at a gasification temperature of 600 ^oC. This was attributed to the reforming of tars and hydrocarbons in the raw product gas in presence of calcium oxide. The CO and CH_4 concentrations in the product gas were lower while using the sorbent. The calcium oxide played the dual role of sorbent and catalyst.

Wang et al. (2008) studied on the effective and economic conversion of the low value and highly distributed solid biomass to a uniform gaseous mixture. Contemporary issues in the thermal gasification of biomass and its application to electricity and fuel production were presented. Steamwas used as the gasifying agent with a product gas heating value of about 10–15 MJ/Nm3, compared to the air gasification of biomass with 3–6 MJ/Nm^3. ER was found to be between 0.2 and 0.4.

Lv et al. (2007) utilized air and oxygen/steam. They found that the maximum lower heating value of fuel gas was 11.11 MJ/Nm^3 and the maximum hydrogen yield reached 45.16 g H_2/kg biomass. For biomass oxygen/steam gasification, the content of H_2 and CO was obtained to be 63.27–72.56%, while the content was 52.19–63.31% for biomass air gasification. The ratio of H_2/CO for biomass oxygen/steam gasification reached 0.7–0.9, which was lower than that of biomass air gasification with 1.06–1.27.

Nikoo and Mahinpey (2008) developed a model for the gasification of biomass in an atmospheric fluidized bed gasifier using the Aspen Plus simulator. The simulation results for the product gas composition and carbon conversion efficiency versus temperature, equivalence ratio (ER), steam to biomass ratio (SBR) and biomass average particle size were compared with the experimental results.

Higher temperature improved the gasification process. It increased both the production of hydrogen and the carbon conversion efficiency. Carbon monoxide and methane showed decreasing trends with increasing the temperature. The CO_2 production and carbon conversion efficiency increased by increasing the ER. In their study, temperatures varied from 700 to 900 ^oC. Biomass feed rate, air and steam rate were obtained to be 0.445–0.512 kg/h, 0.5–0.7 Nm^3/h and 0–1.8 kg/h, respectively.

2.1.1 Drying step

Most gasification systems use dry biomass with moisture contents of 10–20%, in order to generate a high heating value product gas. In this study, a simplified approach is formulated to model drying. It is assumed that the loosely bound water (moisture) present in the biomass irreversibly, instantaneously changes its phase from liquid to gas at a temperature above 100 ^oC. (Kaushal, Abedi, & Mahinpey, 2010)

2.1.2 Devolatilization step

Devolatilization is an extremely complex phenomenon due to the large number of chemical and physical transformation occurring rapidly and simultaneously. In general, when the dried fuel is heated in the range of 200–500 ^oC in absence of oxygen (or any other oxidizing agent), it decomposes into solid char and volatiles (condensable hydrocarbon or tar and gases). This process is called devolatilization. The relative yields of gas and solid depend mostly on the heating-rate and the average temperature. The devolatilization product then reacts with the gasifying medium (air, oxygen or steam) to produce carbon monoxide (CO), carbon dioxide (CO2), hydrogen (H2) and lighter hydrocarbons. (Kaushal, Abedi, & Mahinpey, 2010)

2.1.3 Gasification step

Gasification is achieved at temperatures in excess of 700 ^oC in the presence of oxygen/air and/or steam; however tar free gasification requires much higher temperatures. Syn-gas (CO_2, CO, H_2) is produced when oxygen is used for the gasification as opposed to a producer gas (CO_2, CO, H_2, CH_4, N_2), in which case air is used for gasification. A combination of pyrolysis, partial oxidation and/or steam reforming of gaseous alkanes and char takes place under these conditions. (Tanksale, Beltramini, & Lu, 2010)

The resulting gas, known as producer gas, is a mixture of carbon monoxide, hydrogen and methane, together with carbon dioxide and nitrogen. Yield a product gas from thermal decomposition composed of CO, CO_2, H_2O, H_2, CH_4, other gaseous hydrocarbons (CHs), tars, char, inorganic constituents, and ash. Gas composition of product from the biomass gasification depends heavily on the gasification process, the gasifying agent, and the feedstock composition. (Balat, Balat, Kirtay, & Balat, 2009).

The presence of oxygen or air in the gasification equipment promotes partial oxidation over pyrolysis reactions. Although it is possible to obtain some gaseous products, fast pyrolysis reactions generally produce bio-oils, tar and charcoal. Water gas shift reaction can be conducted in a separate reactor in the presence of CuO–ZnO or Fe catalyst depending upon the reaction temperatures. (Tanksale, Beltramini, & Lu, 2010)

2.1.4 Gas cleaning step

In the work of Florin and Harris (2008), they have reviewed the mechanism of biomass gasification with steam and assessed published work to identify important experimental variables for optimizing H_2 output. However, previous research on the steam gasification of biomass, without CO_2 capture, achieved H_2 concentrations in the product gas of only 40–50%-vol. This output is unlikely to be sufficient for commercial applications.

Thus, in order to increase the H_2 concentration, the use of an in situ CO_2 sorbent was investigated as a technique for boosting H_2 concentration in the product gas. When coupled with CO_2 capture, the output of H_2 from biomass gasification was reported to increase to ~80%-vol.

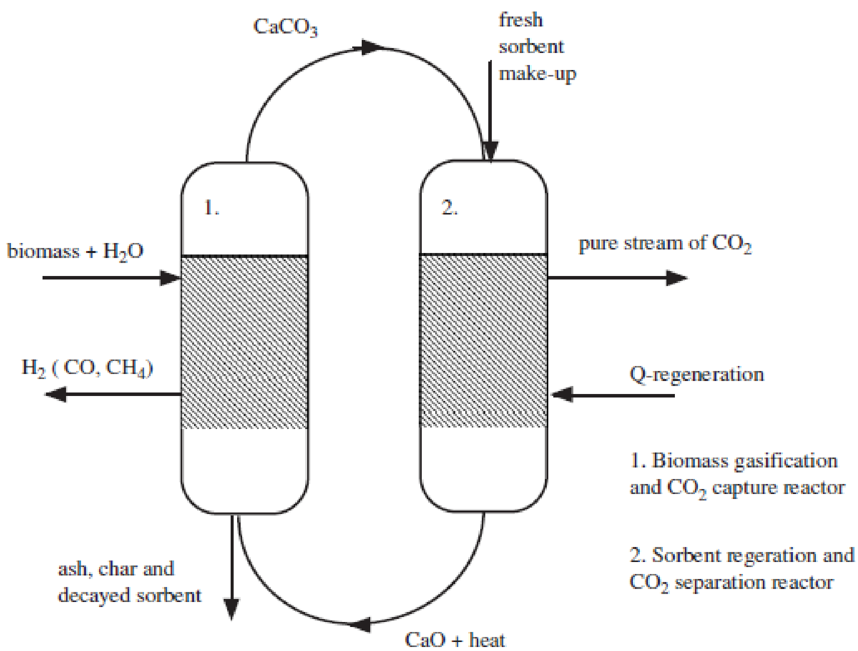

Figure 2 1: Schematic illustration of biomass gasification coupled with CO_2 capture using a CaO sorbent.

In addition, they reported on the performance of CaO-based CO_2 sorbents. They identified significant challenges related to process operability, including: (i) sorbent durability related to resistance to physical deterioration, (ii) incomplete conversion of CaO to $CaCO_3$, and (iii) decay in chemical reactivity when subjected to multiple CO2 capture and release cycles.

They discussed opportunities for enhanced CO_2 capture using optimal calcination conditions, steam hydration treatments and tailored sorbents with CaO embedded in an inert porous matrix. No CaO-based CO_2 sorbent, with demonstrated high reactivity, maintained through multiple CO_2 capture and release cycles, has been identified in the literature. (Florin & Harris, 2008)

2.2 Superstructure optimization of gasification

To complete this superstructure modeling, the simulation data will be extracted from various literatures. For instance, Kaushal et al. (2010) did a comprehensive mathematical model for biomass gasification in a bubbling fluidized bed reactor. The model inputs were reactor geometry, mass flow rate, composition and temperature of incoming streams. The model is capable of predicting the bed temperature, tar yield and, product gas composition, heating value and production rate.

In the journal by Gomez-Barea and Leckner (2010), they performed a review of modeling works on biomass gasification in fluidized bed. It is concluded that most of the fluidized bed biomass gasification models fit reasonably well with the experiments despite the various formulations and input data. In their work, a comparison table was included on literature for modeling of biomass gasification in bubbling fluidized bed reactor. Each literature has model characteristics' which includes type of reactor model, fuel used, the bed temperature, gasification agent and the fluidization agent. The literatures will be narrowed down to ensure only cellulosic biomass is used for the modeling.

Ayoub et al. (2009) reported a superstructure for biomass utilization networks. Biomass utilization network is a group of dependant and interconnected processes for utilizing one or more biomass resources that leads to the production of single or multiple bio-products.

Another previous work on optimization is by Liu et al. (2009) in which a mixed-integer optimization approach is applied for poly-generation systems design. As poly-generation also uses the gasification process to produce power, methanol and hydrogen; the modeling may be extracted to be integrated into the superstructure modeling.

To date, there is limited published work of superstructure optimization of biomass gasification. However, published research on power plants and coal gasification can be used due to this limitation.

CHAPTER 3

METHODOLOGY

3.1 Project Activities

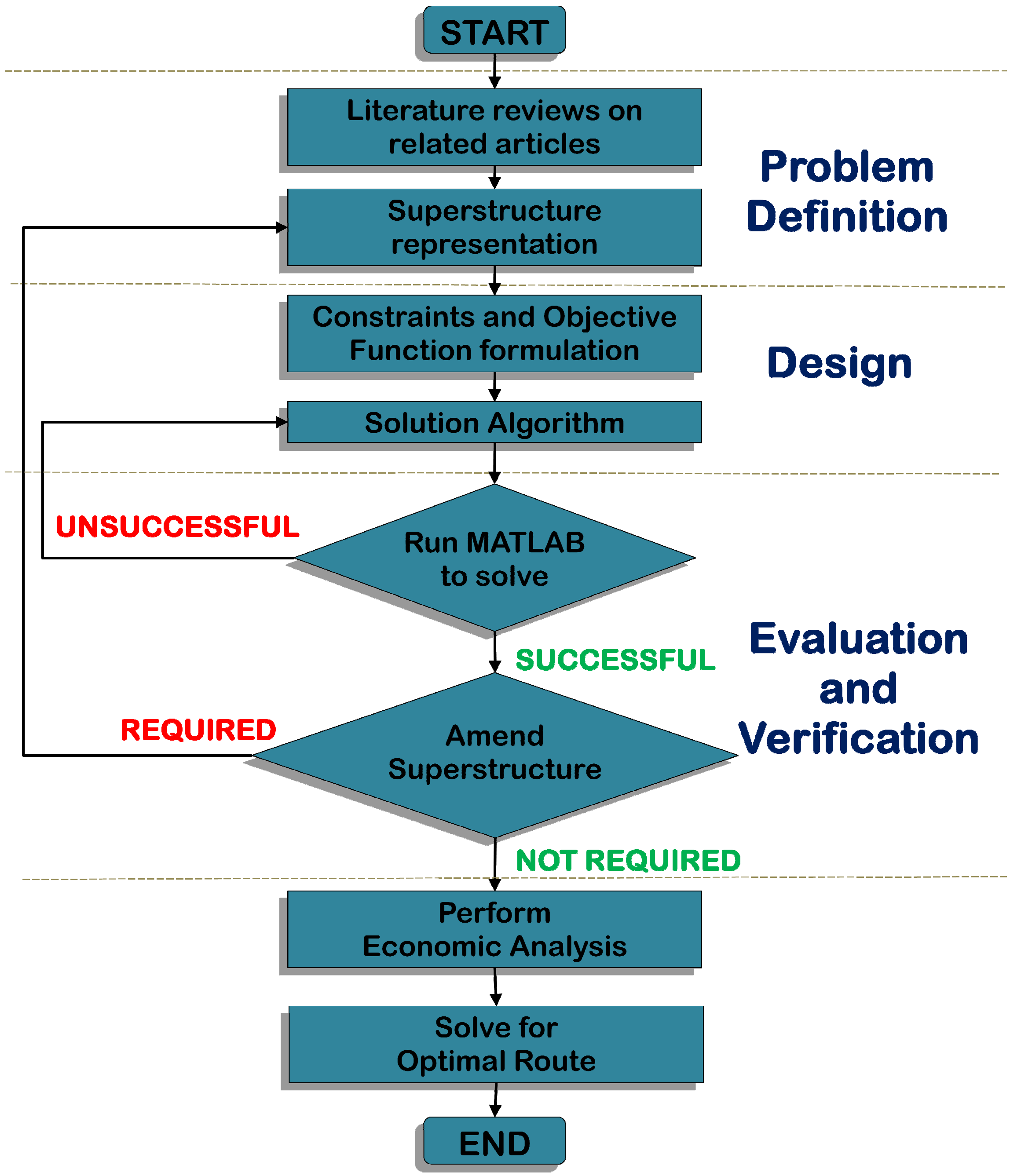

Figure 3.1: Project methodology

There are three basic elements required in development of superstructure optimization methods for process synthesis which are:

3.1.1 Problem representation in superstructure model

The project starts with critical literature review of the production routes of hydrogen from biomass. Upon thorough research, it is narrowed down to general scopes of hydrogen production routes via gasification. This includes the parameters of the reactors/technologies, which are the reactor temperature and pressure, gasification agent, conversion rate for each technology, the pretreatment method and the gas cleaning method. Besides that, the effect of sorbent over biomass ratio and gasification agent over biomass ratio is also taken note. The literature review will give insight and guidance in developing the models to describe the production of hydrogen from biomass via gasification. A superstructure model consisting of all the production routes are integrated into one for easier understanding of the whole model.

Based on the research by Khajehpour et al. (2009), imperfections exist in superstructure models. This is due to the large and complexity of its nature where problem solving tools require a long time to solve. Therefore, reducing the superstructure of study allows faster achievement of feasible results. (Khajehpour, Farhadi, & Pishvaie, 2009) Hence, some variables specified by literature, such as temperature, pressure and ratio of materials, for the feasible routes are eliminated from the superstructure to attain the route with minimal cost faster.

3.1.2 Modeling model formulation and cost minimization

Models of the production routes in the superstructure are developed based on the literature review done on the topic on paper and then, transferred to software. The production route model is compared to the existing models developed in other literatures. Simulations of the models are done using optimization software to obtain the results (MATLAB).

The correlation between the simulation and the data given in the literature is observed. Cost minimization steps are done by reducing the amount of feed intake to yield hydrogen production cost at a lower price.

3.1.3 Search for optimal flowsheet or most feasible route

The relationship between the superstructure simulation and modeling in literature are discussed and any findings are explained. The superstructure simulation is optimized to obtain the feasible route of hydrogen production from biomass via gasification.

3.2 Computational Tools

The Optimization toolbox in MATLAB provides widely used algorithms for standard and large scale optimization. These algorithms solve for discrete and continuous problems. It is suitable for this project as it can be used to find optimal solutions, balance multiple design alternatives and incorporate optimization methods into algorithms and models. For this project, the `fmincon` function is used. This function is used to solve problems relating to types: Continuous, Nonlinear and Constrained

3.4 Gantt Chart

Month	May				June				July					August				
Week	*1*	*2*	*3*	*4*	*1*	*2*	*3*	*4*	*1*	*2*	*3*	*4*	*5*	*1*	*2*	*3*	*4*	*5*
				1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Literature review																		
Data Collection of Feasible Routes																		
Development of Superstructure model																		
Superstructure Simulation																		
Superstructure Optimization																		
Results Validation																		
Achieve optimal route																		
Dissertation																		

Table 3-1: Gantt chart for Final Year Project II

CHAPTER 4:

RESULTS AND DISCUSSION

4.1 Superstructure Model

Numerous technologies and processes are found from literature review. However, the superstructure model is narrowed down for modeling reasons. As each unit and process is simulated in MATLAB, the superstructure model will be added accordingly. Superstructure representation for hydrogen production from biomass is presented here, while Table 4-1 shows the legend for the superstructure representation in Figure 4-1.

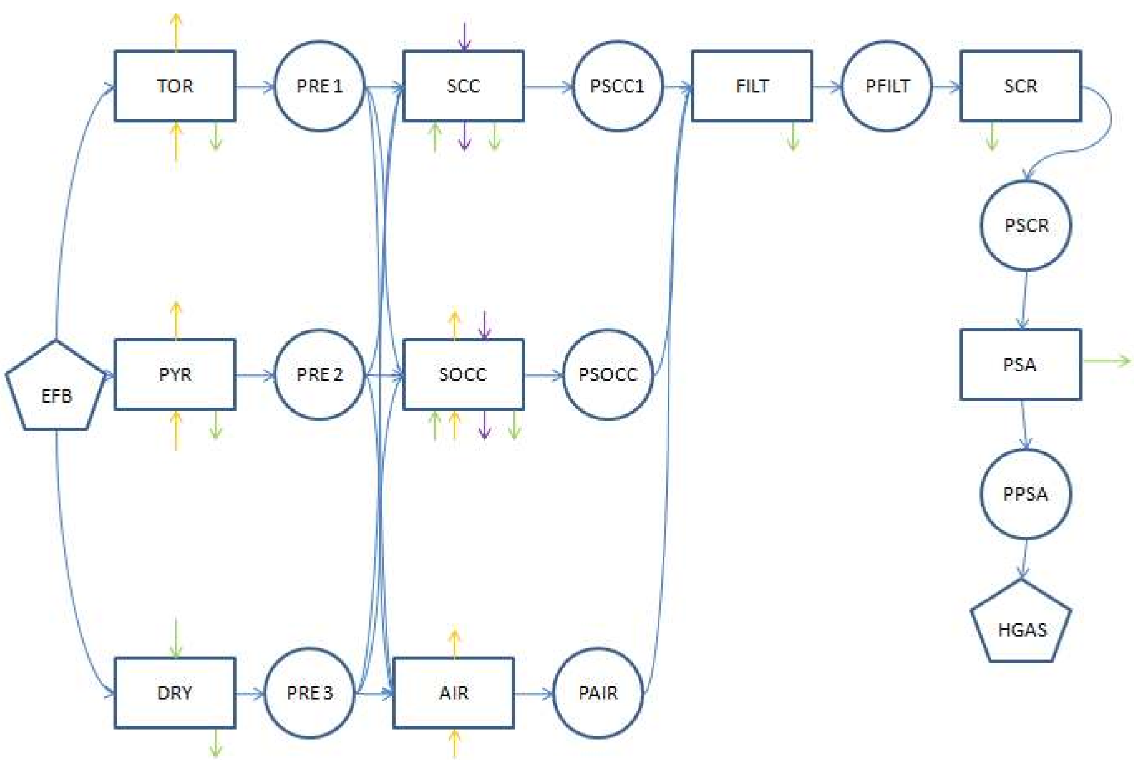

Figure 4-1: Basic superstructure model

Table 4-1: Legend for the superstructure model in Figure 4-1

EFB	Empty Fruit Bunch (Raw Material)
TOR	Torrefaction Reactor
PYR	Pyrolysis Reactor
DRY	Drying Chamber
PRE1	Product Gas of Torrefaction
PRE2	Product Gas of Pyrolysis
PRE3	Product Gas of Drying
SCC	Steam Gasification with Carbon Capture
SOCC	Steam and Oxygen Gasification with Carbon Capture
AIR	Air Gasification
PSCC1	Product Gas of Steam Gasification with Carbon Capture
PSOCC	Product Gas of Steam and Oxygen Gasification with Carbon Capture
PAIR	Product Gas of Air Gasification
FILT	Filter
PFILT	Product Gas of Filter
SCR	Scrubber
PSCR	Product Gas of Scrubber
PSA	Pressure Swing Adsorption
PPSA	Product gas of Presure Swing Adsorption
HGAS	Hydrogen Gas

The finalized methods and technologies taken for the superstructure model are:

a) Pretreatment

   i. Torrefaction (Uemura, N. Omar, Tsutsui, & Yusup, 2011)

   ii. Fast pyrolysis (N, H, & F, 2010)

   iii. Drying using superheated steam (Hasibuan & Wan Daud, 2004)

b) Gasification
    i. Gasification using air (A, A, W A K G, S, & Fakhru'l-Razi, 2011)
    ii. Gasification using steam with carbon capture sorbent (Inayat, Ahmad, Abdul Mutalib, & Yusup, Biomass Steam Gasification with In-Situ CO2 Capture for Enriched Hydrogen Gas Production: A Reaction Kinetics Modelling Approach, 2010), (Florin & Harris, 2008)
    iii. Gasification using steam and oxygen with carbon capture sorbent (Ahmad, Inayat, Abdul Mutalib, & Yusup, 2011), (Florin & Harris, 2008)

c) Gas Cleaning (Inayat, Ahmad, Abdul Mutalib, & Yusup, Flowsheet Modellling of Biomass Steam Gasification System with CO2 Capture for Hydrogen Production, 2010)
    i. Filter
    ii. Scrubber
    iii. Pressure Swing Adsorption

The programming for the superstructure is included in the appendices.

4.2 Optimization Results

Upon running the optimization files, the following results are obtained

a) For Gasification using Air

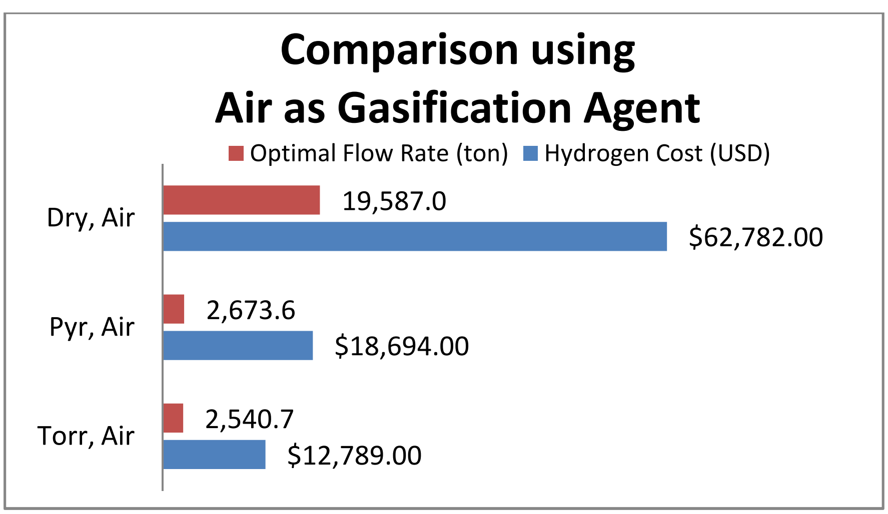

Figure 4.2: Comparison of optimal flow rate and hydrogen cost for routes using air as gasification agent

b) For Gasification using Steam with Carbon Capture Sorbent

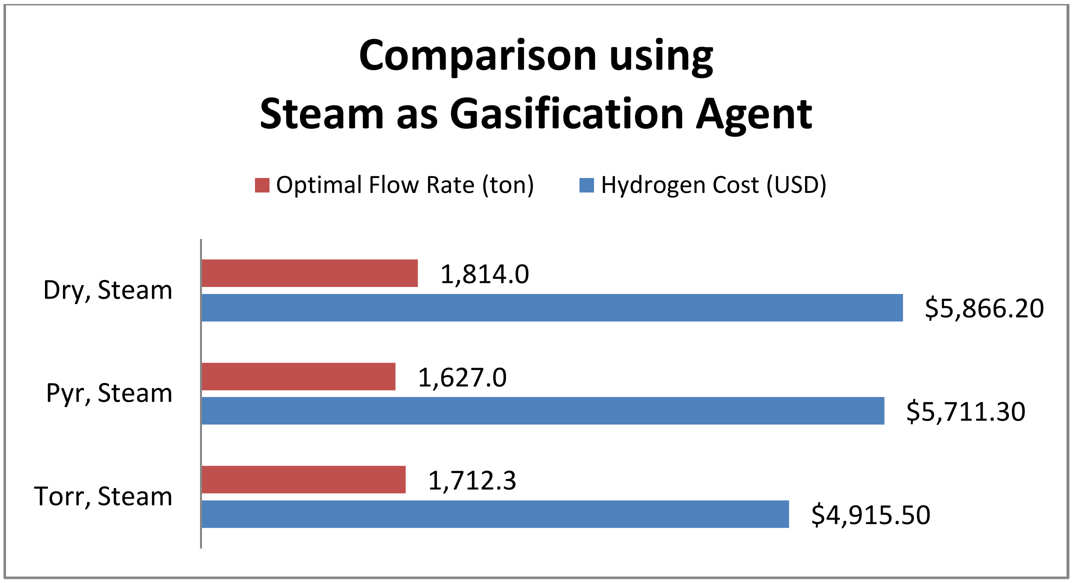

Figure 4.3: Comparison of optimal flow rate and hydrogen cost for routes using steam as gasification agent with CaO sorbent

c) For Gasification using Steam and Oxygen with Carbon Capture Sorbent

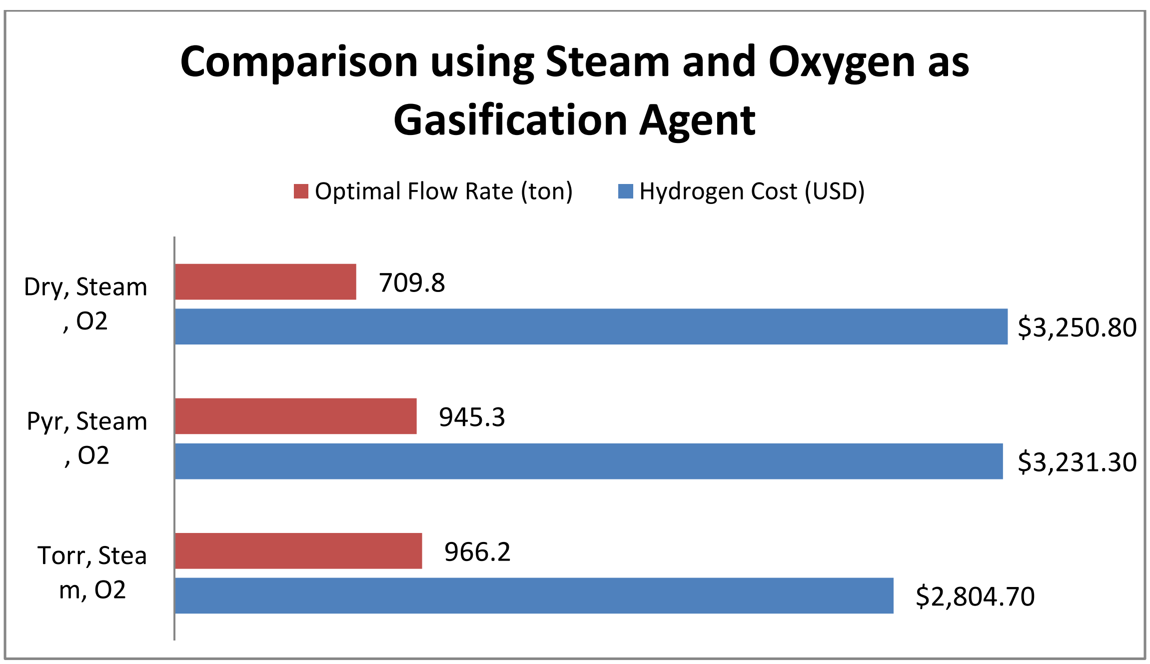

Figure 4.4: Comparison of optimal flow rate and hydrogen cost for routes using steam and oxygen as gasification agent with CaO sorbent

4.3 Results Analysis

Based on the programming results and optimization iterations, only two routes can be analyzed for discussion.

Table 4-2: Comparison of valid results from routes

Route		**Optimal flow rate (EFB) (tonne/yr)**	**Hydrogen Production cost (US$)**
Pre-treatment	Gasification		
Torrefaction	Air	2 540.7	12 789.00
Fast Pyrolysis	Air	2 597.3	18 766.00
Drying using Superheated Steam	Air	19 587	62 782.00
Torrefaction	Steam with Carbon Capture	1 712	4 915.50
Fast Pyrolysis	Steam with Carbon Capture	1 627	5 711.30
Drying using Superheated Steam	Steam with Carbon Capture	1 814	5 866.20
Torrefaction	Steam and Oxygen with Carbon Capture	966	2 804.70
Fast Pyrolysis	Steam and Oxygen with Carbon Capture	945	3 231.30
Drying using Superheated Steam	Steam and Oxygen with Carbon Capture	710	3 250.80

From the table, the higher the optimized value of EFB, the higher the production cost of hydrogen for that route. However, quantitatively, the production route with torrefaction as the pre-treatment process has a lower production cost. This is due to the conversion factor of each process. Torrefaction process has a conversion of 0.4316 (Uemura, N. Omar, Tsutsui, & Yusup, 2011), whilst fast pyrolysis has a maximum conversion of 0.251 (N, H, & F, 2010). The conversion factor is a major factor in calculating the equipment costing and the production costing. This proves that a production technology with a higher conversion rate has the tendency to reduce the hydrogen production cost due to its effectiveness of raw material conversion.

Therefore, the route with the most minimal cost from the optimization model is the route with torrefaction pretreatment and gasification using steam and oxygen with CaO sorbent. However, the production cost of oxygen in a plant is considered. From P. Lv et al. (2008), they approximated a price of US$ 125 057 per year to operate a Pressure Swing Adsorption plant for oxygen purification. From here, it is identified that this model has errors in yielding the price for routes relating with gasification using steam and oxygen with CaO sorbent. Literature also quoted that steam is chosen above steam and oxygen as gasification agents is because it eliminates the necessity of an oxygen plant. (Gao, Li, Quan, & Gao, 2008). Hence, the route with most minimal cost is the route with torrefaction pre-treatment and steam as the gasification agent with CaO sorbent.

4.4 Action Plan

Due to the poor result acquisition, further actions in improving the programming syntax and better analysis will be done in the future to better identify the most cost effective production route once compared with all existing production routes.

CHAPTER 5

CONCLUSION AND RECOMMENDATIONS

5.1 Conclusion

In conclusion, the objectives of this project have been achieved. Firstly, the identification and collection of feasible routes of hydrogen production from biomass via gasification is achieved. Then, followed by the development of the superstructure model in MATLAB, incorporating all variables to determine the optimized value of each variable. The variable is the flow of raw materials, mainly Empty Fruit Bunch (EFB) and the gasification agent (steam, oxygen or both). The constraint involved in the formulation is the minimum hydrogen production cost possible, which greatly involve on the selection of the production route later. This superstructure formulation has further provided an easy and compact representation and visualization of the choices. The optimal configuration obtained is parallel with real operating gasification plants. It has been proven that the superstructure model has successfully achieved the minimum cost (objective function) with optimal flow rate.

5.2 Recommendations

For future work, the model should be more focused on sustainability development of environmental consideration. Thorough studies should be done on the emission factors of the major equipments. Also, the formulation of the emission of gaseous byproducts, such as carbon dioxide (CO2) and carbon monoxide (CO), is to be included in the model. Besides that, the introduction of nonlinearity in the model formulation that takes account the energy balances of the routes can lead to better accuracy of the results.

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APPENDICES

APPENDIX A: PROGRAMMING FILES

<u>Route A</u>: Pretreatment–Torrefaction, Gasification Agent–Air

Route

```
function
[hydrogencost]=calc_hydrogencost
_torrair(X)

[torr_input] =
calc_torrefaction1(X);
[torrair_output] =
calc_air(torr_input);
[torrair_filter_product] =
calc_filter1(torrair_output);
[torrair_scrubber_product] =
calc_scrubber1(torrair_filter_pr
oduct);
[torrair_psa_product] =
calc_psa1(torrair_scrubber_produ
ct);
[total_hydrogen] =
calc_hydrogen1(torrair_psa_produ
ct);

[PEC_torrefaction]=calc_cost_tor
refaction(X);
[PEC_gasifier]=calc_cost_airgasi
fier(torr_input);
[PEC_filter]=calc_cost_filter(to
rrair_output);
[PEC_scrubber]=calc_cost_scrubbe
r(torrair_filter_product);
[PEC_psa]=calc_cost_psa(torrair_
scrubber_product);
[PEC_furnace]=calc_cost_furnance
(torr_input);
[PEC] =
calc_PEC1(PEC_torrefaction,PEC_g
asifier,PEC_filter,PEC_scrubber,
PEC_psa,PEC_furnace);

[FCI] = calc_FCI(PEC);
[TPC] = calc_TPC1(FCI,X);
[TCI] = calc_TCI(FCI);
[hydrogencost] =
calc_hydrogencost(TCI,TPC,total_
hydrogen);

end
```

Route with Constraints

```
function[c,ceq]=calc_hydrogencos
t_torrair_constraints(X)

[torr_input] =
calc_torrefaction1(X);
[torrair_output] =
calc_air(torr_input);
[torrair_filter_product] =
calc_filter1(torrair_output);
[torrair_scrubber_product] =
calc_scrubber1(torrair_filter_pr
oduct);
[torrair_psa_product] =
calc_psa1(torrair_scrubber_produ
ct);
[total_hydrogen] =
calc_hydrogen1(torrair_psa_produ
ct);

[PEC_torrefaction]=calc_cost_tor
refaction(X);
[PEC_gasifier]=calc_cost_airgasi
fier(torr_input);
[PEC_filter]=calc_cost_filter(to
rrair_output);
[PEC_scrubber]=calc_cost_scrubbe
r(torrair_filter_product);
[PEC_psa]=calc_cost_psa(torrair_
scrubber_product);
[PEC_furnace]=calc_cost_furnance
(torr_input);
[PEC] =
calc_PEC1(PEC_torrefaction,PEC_g
asifier,PEC_filter,PEC_scrubber,
PEC_psa,PEC_furnace);

[FCI] = calc_FCI(PEC);
[TPC] = calc_TPC1(FCI,X);
[TCI] = calc_TCI(FCI);
[hydrogencost] =
calc_hydrogencost(TCI,TPC,total_
hydrogen);

ceq=[];
c=2.3-hydrogencost;

end
```

Torrefaction Chamber

```
function [torr_input] =
calc_torrefaction1(efb)
torr_product=efb*0.4316;
torr_input=torr_product;
end
```

Air Gasifier

```
function [output] =
calc_air(input)
air_product=input*0.1;
output=air_product;
end
```

Filter

```
function[torrair_filter_product]
= calc_filter1(torrair_output)
torrair_filter_product=torrair_o
utput*0.963;
end
```

Scrubber

```
function[torrair_scrubber_produc
t] =
calc_scrubber1(torrair_filter_pr
oduct)
torrair_scrubber_product=torrair
_filter_product*0.247;
end
```

Pressure Swing Adsorption Column

```
function[torrair_psa_product] =
calc_psa1(torrair_scrubber_produ
ct)
torrair_psa_product=torrair_scru
bber_product*0.110;
end
```

Amount of Hydrogen Produced

```
function [total_hydrogen] =
calc_hydrogen1(torrair_psa_produ
ct)
total_hydrogen=torrair_psa_produ
ct;
end
```

Cost of Torrefaction Chamber

```
function
[torrefaction_cost]=calc_cost_to
rrefaction(flowrate)
pm=0.49096; % density of EFB
(g/m3)
F=flowrate; % flowrate at
gasifier
k=98.7;
x=0.4316; % based on literature
Uemura
a=F*log(1/(1-x));
b=k*pm;
V=a/b; %volume of gasifier
% L/D =6 (assumed based on
douglas)page 507
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2; % SS
MS=1491.7; %from Chemical
Engineering magazine
torrefaction_cost=(MS/280)*101.9
*(Dr^1.066)*(Lr^0.82)*Fc;
end
```

Cost of Air Gasifier

```
function
[gasifier_cost]=calc_cost_airgas
ifier(flowrate)
pm=0.49096;
F=flowrate;
k=98.7;
x=0.0413;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
gasifier_cost=(MS/280)*101.9*(Dr
^1.066)*(Lr^0.82)*Fc;
end
```

Cost of Filter

```
function
[filter_cost]=calc_cost_filter(f
lowrate)
pm=0.49096;
F=flowrate;
k=98.7;
x=0.963;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
filter_cost=(MS/280)*101.9*(Dr^1
.066)*(Lr^0.82)*Fc;
end
```

Cost of Scrubber

```
function
[scrubber_cost]=calc_cost_scrubb
er(flowrate)
pm=0.49096; % density of EFB
(g/m3)
F=flowrate;
k=98.7;
x=0.138;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
scrubber_cost=(MS/280)*101.9*(Dr
^1.066)*(Lr^0.82)*Fc;
end
```

Cost of Pressure Swing Adsorption Column

```
function
[scrubber_cost]=calc_cost_psa(fl
owrate)
pm=0.49096; % density of EFB
(g/m3)
F=flowrate;
k=98.7;
x=0.110;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
scrubber_cost=(MS/280)*101.9*(Dr
^1.066)*(Lr^0.82)*Fc;
end
```

Cost of Furnace

```
function
[furnance_cost]=calc_cost_furnan
ce(QeeQ)
QeeQ=100;
Q=QeeQ*9.47*10^-10; % energy req
for gasification process QeeQ is
in J/hr and converted to Mbtu/hr
pm=0.49096; % density of EFB
(g/m3)
Fc=1; % based on assumption that
stainless steel materilas
MS=1491.70; %from Chemical
Engineering magazine
furnance_cost=(MS/280)*(5.52*10^
3)*(Q^0.85)*Fc;
end
```

Purchased Equipment Cost

```
function [PEC] =
calc_PEC1(PEC_pretreatment,PEC_f
ilter,PEC_gasifier,PEC_furnace,P
EC_scrubber,PEC_psa)
PEC=PEC_pretreatment+PEC_gasifie
r+PEC_filter+PEC_furnace+PEC_scr
ubber+PEC_psa;
end
```

Fixed Capital Investment

```
function [FCI] = calc_FCI(PEC)
DC=3.778*PEC;
IC=0.4165*PEC;
FCI=DC+IC;
end
```

Total Production Cost

```
function [TPC] =
calc_TPC1(FCI,efb)
rawcost=efb*0.015; % Assuming
efb in kg/hr and efb costs USD
0.015/kg
utility=12.90; % USD 12.90/kg.
Taken from P. Lv et al.
catalystcost=efb*7.8279; % USD
7.8279/kg.  Taken from P. Lv et
al.
sorbentcost=efb*0.098; % USD
0.098/kg. Taken from iCheme
Website, 2002
OL=0.15*FCI;
supervision=0.15*OL;
repair=0.05*FCI;
TDPC=rawcost+utility+catalystcos
t+sorbentcost+OL+supervision+rep
air;
TPC=TDPC;
end
```

Total Capital Investment

```
function [TCI] = calc_TCI(FCI)
WC=0.2*FCI;
TCI=FCI+WC;
end
```

Cost of Hydrogen Produced

```
function [hydrogencost] =
calc_hydrogencost(TCI,TPC,total_
hydrogen)
TC=TCI+TPC;
hydrogencost=TC/total_hydrogen;
end
```

Optimization

```
% define the initial guess
independent variables for
optimization
X0=1;
% define the lower bounds for
independent variables
LB=[];
% define the upper bounds for
independent variables
UB=[];
% define the coefficients for
the linear inequality
constraints
A = [];
B = [];
% define the coefficients for
the linear equality constraints
Aeq = [];
Beq = [];
% define the options for the
optimization solver
options =
optimset('Algorithm','active-
set','Display',
'iter','MaxFunEvals',1e6,'MaxIte
r',1e6, ...
    'TolFun',1e-
6,'TolConSQP',1e-6,'TolX',1e-
6,'FunValCheck','on');
% solving the optimization
problem
[X,FVAL,EXITFLAG,OUTPUT,LAMBDA,G
RAD,HESSIAN]=fmincon(@calc_hydro
gencost_torrair,X0,A,B,Aeq,Beq,L
B,UB,@calc_hydrogencost_torrair_
constraints,options);
```

<u>Route B</u>: Pretreatment–Torrefaction, Gasification Agent–Steam with Carbon Capture

Route

```
function[hydrogencost]=calc_hydr
ogencost_torrscc(X)

[torr_input] =
calc_torrefaction(X);
[torrscc_output,steamflow] =
calc_scc(torr_input);
[torrscc_filter_product] =
calc_filter(torrscc_output);
[torrscc_scrubber_product] =
calc_scrubber(torrscc_filter_pro
duct);
[torrscc_psa_product] =
calc_psa(torrscc_scrubber_produc
t);
[total_hydrogen] =
calc_hydrogen(torrscc_psa_produc
t);
```

```
[PEC_torrefaction]=calc_cost_tor
refaction(X);
[PEC_gasifier]=calc_cost_sccgasi
fier(torr_input);
[PEC_filter]=calc_cost_filter(to
rrscc_output);
[PEC_scrubber]=calc_cost_scrubbe
r(torrscc_filter_product);
[PEC_psa]=calc_cost_psa(torrscc_
scrubber_product);
[PEC_furnace]=calc_cost_furnance
(torr_input);
[PEC_boiler]=calc_cost_boiler(st
eamflow);
[PEC] =
calc_PEC2(PEC_torrefaction,PEC_g
asifier,PEC_filter,PEC_scrubber,
PEC_psa,PEC_furnace,PEC_boiler);

[FCI] = calc_FCI(PEC);
[TPC] =
calc_TPC(FCI,X,steamflow);
[TCI] = calc_TCI(FCI);
[hydrogencost] =
calc_hydrogencost(TCI,TPC,total_
hydrogen);

end
```

Route with Constraints

```
function[c,ceq]=calc_hydrogencos
t_torrscc_constraints(X)

[torr_input] =
calc_torrefaction(X);
[torrscc_output,steamflow] =
calc_scc(torr_input);
[torrscc_filter_product] =
calc_filter(torrscc_output);
[torrscc_scrubber_product] =
calc_scrubber(torrscc_filter_pro
duct);
[torrscc_psa_product] =
calc_psa(torrscc_scrubber_produc
t);
[total_hydrogen] =
calc_hydrogen(torrscc_psa_produc
t);

[PEC_torrefaction]=calc_cost_tor
refaction(X);
[PEC_gasifier]=calc_cost_sccgasi
fier(torr_input);
[PEC_filter]=calc_cost_filter(to
rrscc_output);
[PEC_scrubber]=calc_cost_scrubbe
r(torrscc_filter_product);
[PEC_psa]=calc_cost_psa(torrscc_
scrubber_product);
[PEC_furnace]=calc_cost_furnance
(torr_input);
[PEC_boiler]=calc_cost_boiler(st
eamflow);
[PEC] =
calc_PEC2(PEC_torrefaction,PEC_g
asifier,PEC_filter,PEC_scrubber,
PEC_psa,PEC_furnace,PEC_boiler);

[FCI] = calc_FCI(PEC);
[TPC] =
calc_TPC(FCI,X,steamflow);
[TCI] = calc_TCI(FCI);
[hydrogencost] =
calc_hydrogencost(TCI,TPC,total_
hydrogen);

ceq=[];
c=2.3-hydrogencost;

end
```

Torrefaction Chamber

```
function [input] =
calc_torrefaction(efb)
torr_product=efb*0.4316;
input=torr_product;
end
```

Steam Gasification with Carbon Capture

```
function[output,steamflow] =
calc_scc(input)
steamflow=input*3;
product=input*3.54;
output=product;
end
```

Filter

```
function [filter_product] =
calc_filter(output)
filter_product=output*0.963;
end
```

Scrubber

```
function [scrubber_product] =
calc_scrubber(filter_product)
scrubber_product=filter_product*
0.247;
end
```

Pressure Swing Adsorption Column

```
function [psa_product] =
calc_psa(filter_product)
psa_product=filter_product*0.110
;
end
```

Amount of Hydrogen Produced

```
function [total_hydrogen] =
calc_hydrogen(psa_byproduct)
total_hydrogen=psa_byproduct;
end
```

Cost of Torrefaction Chamber

```
function
[torrefaction_cost]=calc_cost_to
rrefaction(flowrate)
pm=0.49096; % density of EFB
(g/m3)
F=flowrate; % flowrate at
gasifier
k=98.7;
x=0.4316; % based on literature
Uemura
a=F*log(1/(1-x));
b=k*pm;
V=a/b; %volume of gasifier
% L/D =6 (assumed based on
douglas)page 507
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2; % SS
MS=1491.7; %from Chemical
Engineering magazine
torrefaction_cost=(MS/280)*101.9
*(Dr^1.066)*(Lr^0.82)*Fc;
end
```

Cost of Steam Gasification with Carbon Capture

```
function
[gasifier_cost]=calc_cost_sccgas
ifier(flowrate)
pm=0.49096;
F=flowrate;
k=98.7;
x=0.708;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
gasifier_cost=(MS/280)*101.9*(Dr
^1.066)*(Lr^0.82)*Fc;
end
```

Cost of Filter

```
function
[filter_cost]=calc_cost_filter(f
lowrate)
pm=0.49096;
F=flowrate;
k=98.7;
x=0.963;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
filter_cost=(MS/280)*101.9*(Dr^1
.066)*(Lr^0.82)*Fc;
end
```

Cost of Scrubber

```
function
[scrubber_cost]=calc_cost_scrubb
er(flowrate)
pm=0.49096; % density of EFB
(g/m3)
F=flowrate;
k=98.7;
x=0.138;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
scrubber_cost=(MS/280)*101.9*(Dr
^1.066)*(Lr^0.82)*Fc;
end
```

Cost of Pressure Swing Adsorption

```
function
[scrubber_cost]=calc_cost_psa(fl
owrate)
pm=0.49096; % density of EFB
(g/m3)
F=flowrate;
k=98.7;
x=0.110;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
scrubber_cost=(MS/280)*101.9*(Dr
^1.066)*(Lr^0.82)*Fc;
end
```

Cost of Furnace

```
function
[furnance_cost]=calc_cost_furnan
ce(QeeQ)
QeeQ=100;
Q=QeeQ*9.47*10^-10; % energy req
for gasification process QeeQ is
in J/hr and converted to Mbtu/hr
pm=0.49096; % density of EFB
(g/m3)
Fc=1; % based on assumption that
stainless steel materilas
MS=1491.70; %from Chemical
Engineering magazine
furnance_cost=(MS/280)*(5.52*10^
3)*(Q^0.85)*Fc;
end
```

Cost of Boiler

```
function
[boiler_cost]=calc_cost_boiler(s
teamflow)
ST=steamflow;
MD=1000;
boiler_cost=(3.28*10^5)*(ST/MD)^
0.81;
end
```

Purchased Equipment Cost

```
function [PEC] =
calc_PEC2(PEC_pretreatment,PEC_g
asifier,PEC_filter,PEC_scrubber,
PEC_psa,PEC_furnace,PEC_boiler)
PEC=PEC_pretreatment+PEC_gasifie
r+PEC_filter+PEC_scrubber+PEC_ps
a+PEC_furnace+PEC_boiler;
end
```

Fixed Capital Investment

```
function [FCI] = calc_FCI(PEC)
DC=3.778*PEC;
IC=0.4165*PEC;
FCI=DC+IC;
end
```

Total Production Cost

```
function [TPC] =
calc_TPC(FCI,efb,steamflow)
rawcost=efb*0.015; % Assuming
efb in kg/hr and efb costs USD
0.015/kg
utility=12.90; % USD 12.90/kg.
Taken from P. Lv et al.
steamcost=steamflow*0.002; % USD
0.002/kg. Taken from Hamada
Boiler Malaysia, 2008
```

```
catalystcost=efb*7.8279; % USD
7.8279/kg.  Taken from P. Lv et
al.
sorbentcost=efb*0.098; % USD
0.098/kg. Taken from iCheme
Website, 2002
OL=0.15*FCI;
supervision=0.15*OL;
repair=0.05*FCI;
TDPC=rawcost+utility+steamcost+c
atalystcost+sorbentcost+OL+super
vision+repair;
TPC=TDPC;
end
```

Total Capital Investment

```
function [TCI] = calc_TCI(FCI)
WC=0.2*FCI;
TCI=FCI+WC;
end
```

Cost of Hydrogen Produced

```
function [hydrogencost] =
calc_hydrogencost(TCI,TPC,total_
hydrogen)
TC=TCI+TPC;
hydrogencost=TC/total_hydrogen;
end
```

Optimization

```
% define the initial guess
independent variables for
optimization
X0=1;
% define the lower bounds for
independent variables
LB=[];
% define the upper bounds for
independent variables
UB=[];
% define the coefficients for
the linear inequality
constraints
A = [];
B = [];
% define the coefficients for
the linear equality constraints
Aeq = [];
Beq = [];
% define the options for the
optimization solver
options =
optimset('Algorithm','active-
set','Display',
'iter','MaxFunEvals',1e6,'MaxIte
r',1e6, ...
    'TolFun',1e-
6,'TolConSQP',1e-6,'TolX',1e-
6,'FunValCheck','on');
% solving the optimization
problem
[X,FVAL,EXITFLAG,OUTPUT,LAMBDA,G
RAD,HESSIAN]=fmincon(@calc_hydro
gencost_torrscc,X0,A,B,Aeq,Beq,L
B,UB,@calc_hydrogencost_torrscc_
constraints,options);
```

<u>Route C</u>: Pretreatment–Torrefaction, Gasification Agent–Steam and Oxygen with Carbon Capture

Route

```
function[hydrogencost]=calc_hydr
ogencost_torrsocc(X)

[torr_input] =
calc_torrefaction(X);
[torrsocc_output,steamflow] =
calc_socc(torr_input);
[torrsocc_filter_product] =
calc_filter(torrsocc_output);
[torrsocc_scrubber_product] =
calc_scrubber(torrsocc_filter_pr
oduct);
[torrsocc_psa_product] =
calc_psa(torrsocc_scrubber_produ
ct);
[total_hydrogen] =
calc_hydrogen(torrsocc_psa_produ
ct);

[PEC_torrefaction]=calc_cost_tor
refaction(X);
[PEC_gasifier]=calc_cost_soccgas
ifier(torr_input);
[PEC_filter]=calc_cost_filter(to
rrsocc_output);
[PEC_scrubber]=calc_cost_scrubbe
r(torrsocc_filter_product);
[PEC_psa]=calc_cost_psa(torrsocc
_scrubber_product);
[PEC_furnace]=calc_cost_furnance
(torr_input);
```

```
[PEC_boiler]=calc_cost_boiler(st
eamflow);
[PEC] =
calc_PEC2(PEC_torrefaction,PEC_g
asifier,PEC_filter,PEC_scrubber,
PEC_psa,PEC_furnace,PEC_boiler);

[FCI] = calc_FCI(PEC);
[TPC] =
calc_TPC(FCI,X,steamflow);
[TCI] = calc_TCI(FCI);
[hydrogencost] =
calc_hydrogencost(TCI,TPC,total_
hydrogen);

end
```

Route with Constraints

```
function[c,ceq]=calc_hydrogencos
t_torrsocc_constraints(X)

[torr_input] =
calc_torrefaction(X);
[torrsocc_output,steamflow] =
calc_socc(torr_input);
[torrsocc_filter_product] =
calc_filter(torrsocc_output);
[torrsocc_scrubber_product] =
calc_scrubber(torrsocc_filter_pr
oduct);
[torrsocc_psa_product] =
calc_psa(torrsocc_scrubber_produ
ct);
[total_hydrogen] =
calc_hydrogen(torrsocc_psa_produ
ct);

[PEC_torrefaction]=calc_cost_tor
refaction(X);
[PEC_gasifier]=calc_cost_soccgas
ifier(torr_input);
[PEC_filter]=calc_cost_filter(to
rrsocc_output);
[PEC_scrubber]=calc_cost_scrubbe
r(torrsocc_filter_product);
[PEC_psa]=calc_cost_psa(torrsocc
_scrubber_product);
[PEC_furnace]=calc_cost_furnance
(torr_input);
[PEC_boiler]=calc_cost_boiler(st
eamflow);
[PEC] =
calc_PEC2(PEC_torrefaction,PEC_g
asifier,PEC_filter,PEC_scrubber,
PEC_psa,PEC_furnace,PEC_boiler);

[FCI] = calc_FCI(PEC);
[TPC] =
calc_TPC(FCI,X,steamflow);
[TCI] = calc_TCI(FCI);
[hydrogencost] =
calc_hydrogencost(TCI,TPC,total_
hydrogen);

ceq=[];
c=2.3-hydrogencost;

end
```

Torrefaction Chamber

```
function [input] =
calc_torrefaction(efb)
torr_product=efb*0.4316;
input=torr_product;
end
```

Steam with Gasification with Carbon Capture

```
function [output,socc_steamflow]
= calc_socc(input)
socc_steamflow=input*4.342;
socc_product=input*9.708;
output=socc_product;
end
```

Filter

```
function [filter_product] =
calc_filter(output)
filter_product=output*0.963;
end
```

Scrubber

```
function [scrubber_product] =
calc_scrubber(filter_product)
scrubber_product=filter_product*
0.247;
end
```

Pressure Swing Adsorption Column

```
function [psa_product] =
calc_psa(filter_product)
psa_product=filter_product*0.110
;
end
```

Amount of Hydrogen Produced

```
function [total_hydrogen] =
calc_hydrogen(psa_byproduct)
total_hydrogen=psa_byproduct;
end
```

Cost of Torrefaction Chamber

```
function
[torrefaction_cost]=calc_cost_to
rrefaction(flowrate)
pm=0.49096; % density of EFB
(g/m3)
F=flowrate; % flowrate at
gasifier
k=98.7;
x=0.4316; % based on literature
Uemura
a=F*log(1/(1-x));
b=k*pm;
V=a/b; %volume of gasifier
% L/D =6 (assumed based on
douglas)page 507
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2; % SS
MS=1491.7; %from Chemical
Engineering magazine
torrefaction_cost=(MS/280)*101.9
*(Dr^1.066)*(Lr^0.82)*Fc;
end
```

Cost of Steam with Oxygen Gasification

with Carbon Capture

```
function
[gasifier_cost]=calc_cost_soccga
sifier(flowrate)
pm=0.49096;
F=flowrate;
k=98.7;
x=0.761;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
gasifier_cost=(MS/280)*101.9*(Dr
^1.066)*(Lr^0.82)*Fc;
end
```

Cost of Filter

```
function
[filter_cost]=calc_cost_filter(f
lowrate)
pm=0.49096;
F=flowrate;
k=98.7;
x=0.963;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
filter_cost=(MS/280)*101.9*(Dr^1
.066)*(Lr^0.82)*Fc;
end
```

Cost of Scrubber

```
function
[scrubber_cost]=calc_cost_scrubb
er(flowrate)
pm=0.49096; % density of EFB
(g/m3)
F=flowrate;
k=98.7;
x=0.138;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
```

```
scrubber_cost=(MS/280)*101.9*(Dr
^1.066)*(Lr^0.82)*Fc;
end
```

Cost of Pressure Swing Adsorption

```
function
[scrubber_cost]=calc_cost_psa(fl
owrate)
pm=0.49096; % density of EFB
(g/m3)
F=flowrate;
k=98.7;
x=0.110;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
scrubber_cost=(MS/280)*101.9*(Dr
^1.066)*(Lr^0.82)*Fc;
end
```

Cost of Furnace

```
function
[furnance_cost]=calc_cost_furnan
ce(QeeQ)
QeeQ=100;
Q=QeeQ*9.47*10^-10; % energy req
for gasification process QeeQ is
in J/hr and converted to Mbtu/hr
pm=0.49096; % density of EFB
(g/m3)
Fc=1; % based on assumption that
stainless steel materilas
MS=1491.70; %from Chemical
Engineering magazine
furnance_cost=(MS/280)*(5.52*10^
3)*(Q^0.85)*Fc;
end
```

Cost of Boiler

```
function
[boiler_cost]=calc_cost_boiler(s
teamflow)
ST=steamflow;
MD=1000;
boiler_cost=(3.28*10^5)*(ST/MD)^
0.81;
end
```

Purchased Equipment Cost

```
function [PEC] =
calc_PEC2(PEC_pretreatment,PEC_g
asifier,PEC_filter,PEC_scrubber,
PEC_psa,PEC_furnace,PEC_boiler)
PEC=PEC_pretreatment+PEC_gasifie
r+PEC_filter+PEC_scrubber+PEC_ps
a+PEC_furnace+PEC_boiler;
end
```

Fixed Capital Investment

```
function [FCI] = calc_FCI(PEC)
DC=3.778*PEC;
IC=0.4165*PEC;
FCI=DC+IC;
end
```

Total Production Cost

```
function [TPC] =
calc_TPC(FCI,efb,steamflow)
rawcost=efb*0.015; % Assuming
efb in kg/hr and efb costs USD
0.015/kg
utility=12.90; % USD 12.90/kg.
Taken from P. Lv et al.
steamcost=steamflow*0.002; % USD
0.002/kg. Taken from Hamada
Boiler Malaysia, 2008
catalystcost=efb*7.8279; % USD
7.8279/kg.  Taken from P. Lv et
al.
sorbentcost=efb*0.098; % USD
0.098/kg. Taken from iCheme
Website, 2002
OL=0.15*FCI;
supervision=0.15*OL;
repair=0.05*FCI;
TDPC=rawcost+utility+steamcost+c
atalystcost+sorbentcost+OL+super
vision+repair;
TPC=TDPC;
end
```

Total Capital Investment

```
function [TCI] = calc_TCI(FCI)
WC=0.2*FCI;
TCI=FCI+WC;
end
```

Cost of Hydrogen Produced

```
function [hydrogencost] =
calc_hydrogencost(TCI,TPC,total_
hydrogen)
TC=TCI+TPC;
hydrogencost=TC/total_hydrogen;
end
```

Optimization

```
% define the initial guess
independent variables for
optimization
X0=1;
% define the lower bounds for
independent variables
LB=[];
% define the upper bounds for
independent variables
UB=[];
% define the coefficients for
the linear inequality
constraints
A = [];
B = [];
% define the coefficients for
the linear equality constraints
Aeq = [];
Beq = [];
% define the options for the
optimization solver
options =
optimset('Algorithm','active-
set','Display',
'iter','MaxFunEvals',1e6,'MaxIte
r',1e6, ...
    'TolFun',1e-
6,'TolConSQP',1e-6,'TolX',1e-
6,'FunValCheck','on');
% solving the optimization
problem
[X,FVAL,EXITFLAG,OUTPUT,LAMBDA,G
RAD,HESSIAN]=fmincon(@calc_hydro
gencost_torrsocc,X0,A,B,Aeq,Beq,
LB,UB,@calc_hydrogencost_torrsoc
c_constraints,options);
```

Route D: Pretreatment–Fast Pyrolysis, Gasification Agent–Air

Route

```
function[hydrogencost]=calc_hydr
ogencost_pyrair(X)

[pyr_input] = calc_pyrolysis(X);
[pyrair_output] =
calc_air(pyr_input);
[pyrair_filter_product] =
calc_filter(pyrair_output);
[pyrair_scrubber_product] =
calc_scrubber(pyrair_filter_prod
uct);
[pyrair_psa_product] =
calc_psa(pyrair_scrubber_product
);
[total_hydrogen] =
calc_hydrogen(pyrair_psa_product
);

[PEC_pyrolysis]=calc_cost_pyroly
sis(X);
[PEC_gasifier]=calc_cost_airgasi
fier(pyr_input);
[PEC_filter]=calc_cost_filter(py
rair_output);
[PEC_scrubber]=calc_cost_scrubbe
r(pyrair_filter_product);
[PEC_psa]=calc_cost_psa(pyrair_s
crubber_product);
[PEC_furnace]=calc_cost_furnance
(pyr_input);
[PEC] =
calc_PEC1(PEC_pyrolysis,PEC_gasi
fier,PEC_filter,PEC_scrubber,PEC
_psa,PEC_furnace);

[FCI] = calc_FCI(PEC);
[TPC] = calc_TPC1(FCI,X);
[TCI] = calc_TCI(FCI);
[hydrogencost] =
calc_hydrogencost(TCI,TPC,total_
hydrogen);

end
```

Route with Constraints

```
function[c,ceq]=calc_hydrogencos
t_pyrair_constraints(X)

[pyr_input] = calc_pyrolysis(X);
[pyrair_output] =
calc_air(pyr_input);
[pyrair_filter_product] =
calc_filter(pyrair_output);
[pyrair_scrubber_product] =
calc_scrubber(pyrair_filter_prod
uct);
[pyrair_psa_product] =
calc_psa(pyrair_scrubber_product
);
[total_hydrogen] =
calc_hydrogen(pyrair_psa_product
);

[PEC_pyrolysis]=calc_cost_pyroly
sis(X);
[PEC_gasifier]=calc_cost_airgasi
fier(pyr_input);
[PEC_filter]=calc_cost_filter(py
rair_output);
[PEC_scrubber]=calc_cost_scrubbe
r(pyrair_filter_product);
[PEC_psa]=calc_cost_psa(pyrair_s
crubber_product);
[PEC_furnace]=calc_cost_furnance
(pyr_input);
[PEC] =
calc_PEC1(PEC_pyrolysis,PEC_gasi
fier,PEC_filter,PEC_scrubber,PEC
_psa,PEC_furnace);

[FCI] = calc_FCI(PEC);
[TPC] = calc_TPC1(FCI,X);
[TCI] = calc_TCI(FCI);
[hydrogencost] =
calc_hydrogencost(TCI,TPC,total_
hydrogen);

ceq=[];
c=2.3-hydrogencost;

end
```

Fast Pyrolysis Chamber

```
function [pyr_input] =
calc_pyrolysis(efb)
pyr_char=efb*0.251;
pyr_input=pyr_char;
end
```

Air Gasification

```
function [output] =
calc_air(input)
air_product=input*0.1;
output=air_product;
end
```

Filter

```
function [filter_product] =
calc_filter(output)
filter_product=output*0.963;
end
```

Scrubber

```
function [scrubber_product] =
calc_scrubber(filter_product)
scrubber_product=filter_product*
0.247;
end
```

Pressure Swing Adsorption Column

```
function [psa_product] =
calc_psa(filter_product)
psa_product=filter_product*0.110
;
end
```

Amount of Hydrogen Produced

```
function [total_hydrogen] =
calc_hydrogen(psa_byproduct)
total_hydrogen=psa_byproduct;
end
```

Cost of Fast Pyrolysis Chamber

```
function
[pyrolysis_cost]=calc_cost_pyrol
ysis(flowrate)
pm=0.49096; % density of EFB
(g/m3)
F=flowrate; % flowrate at
gasifier
k=98.7;
x=0.251;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2; % SS
MS=1491.7;
pyrolysis_cost=(MS/280)*101.9*(D
r^1.066)*(Lr^0.82)*Fc;
end
```

Cost of Air Gasification

```
function
[gasifier_cost]=calc_cost_airgas
ifier(flowrate)
pm=0.49096;
F=flowrate;
k=98.7;
x=0.0413;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
gasifier_cost=(MS/280)*101.9*(Dr
^1.066)*(Lr^0.82)*Fc;
end
```

Cost of Filter

```
function
[filter_cost]=calc_cost_filter(f
lowrate)
pm=0.49096;
F=flowrate;
k=98.7;
x=0.963;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
filter_cost=(MS/280)*101.9*(Dr^1
.066)*(Lr^0.82)*Fc;
end
```

Cost of Scrubber

```
function
[scrubber_cost]=calc_cost_scrubb
er(flowrate)
pm=0.49096; % density of EFB
(g/m3)
F=flowrate;
k=98.7;
x=0.138;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
scrubber_cost=(MS/280)*101.9*(Dr
^1.066)*(Lr^0.82)*Fc;
end
```

Cost of Pressure Swing Adsorption

```
function
[scrubber_cost]=calc_cost_psa(fl
owrate)
pm=0.49096; % density of EFB
(g/m3)
F=flowrate;
k=98.7;
x=0.110;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
```

```
scrubber_cost=(MS/280)*101.9*(Dr
^1.066)*(Lr^0.82)*Fc;
end
```

Cost of Furnace

```
function
[furnance_cost]=calc_cost_furnan
ce(QeeQ)
QeeQ=100;
Q=QeeQ*9.47*10^-10; % energy req
for gasification process QeeQ is
in J/hr and converted to Mbtu/hr
pm=0.49096; % density of EFB
(g/m3)
Fc=1; % based on assumption that
stainless steel materilas
MS=1491.70; %from Chemical
Engineering magazine
furnance_cost=(MS/280)*(5.52*10^
3)*(Q^0.85)*Fc;
end
```

Purchased Equipment Cost

```
function [PEC] =
calc_PEC1(PEC_pretreatment,PEC_f
ilter,PEC_gasifier,PEC_furnace,P
EC_scrubber,PEC_psa)
PEC=PEC_pretreatment+PEC_gasifie
r+PEC_filter+PEC_furnace+PEC_scr
ubber+PEC_psa;
end
```

Fixed Capital Investment

```
function [FCI] = calc_FCI(PEC)
DC=3.778*PEC;
IC=0.4165*PEC;
FCI=DC+IC;
end
```

Total Production Cost

```
function [TPC] =
calc_TPC1(FCI,efb)
rawcost=efb*0.015; % Assuming
efb in kg/hr and efb costs USD
0.015/kg
utility=12.90; % USD 12.90/kg.
Taken from P. Lv et al.
catalystcost=efb*7.8279; % USD
7.8279/kg.  Taken from P. Lv et
al.
sorbentcost=efb*0.098; % USD
0.098/kg. Taken from iCheme
Website, 2002
OL=0.15*FCI;
supervision=0.15*OL;
repair=0.05*FCI;
TDPC=rawcost+utility+catalystcos
t+sorbentcost+OL+supervision+rep
air;
TPC=TDPC;
end
```

Total Capital Investment

```
function [TCI] = calc_TCI(FCI)
WC=0.2*FCI;
TCI=FCI+WC;
end
```

Cost of Hydrogen Produced

```
function [hydrogencost] =
calc_hydrogencost(TCI,TPC,total_
hydrogen)
TC=TCI+TPC;
hydrogencost=TC/total_hydrogen;
end
```

Optimization

```
% define the initial guess
independent variables for
optimization
X0=1;
% define the lower bounds for
independent variables
LB=[];
% define the upper bounds for
independent variables
UB=[];
% define the coefficients for
the linear inequality
constraints
A = [];
B = [];
% define the coefficients for
the linear equality constraints
Aeq = [];
Beq = [];
% define the options for the
optimization solver
options =
optimset('Algorithm','active-
set','Display',
```

```
'iter','MaxFunEvals',1e6,'MaxIte
r',1e6, ...
    'TolFun',1e-
6,'TolConSQP',1e-6,'TolX',1e-
6,'FunValCheck','on');
% solving the optimization
problem
[X,FVAL,EXITFLAG,OUTPUT,LAMBDA,G
RAD,HESSIAN]=fmincon(@calc_hydro
gencost_pyrair,X0,A,B,Aeq,Beq,LB
,UB,@calc_hydrogencost_pyrair_co
nstraints,options);
```

<u>Route E</u>: Pretreatment–Fast Pyrolysis, Gasification Agent–Steam with Carbon Capture

Route

```
function[hydrogencost]=calc_hydr
ogencost_pyrscc(X)

[pyr_input] = calc_pyrolysis(X);
[pyrscc_output,steamflow] =
calc_scc(pyr_input);
[pyrscc_filter_product] =
calc_filter(pyrscc_output);
[pyrscc_scrubber_product] =
calc_scrubber(pyrscc_filter_prod
uct);
[pyrscc_psa_product] =
calc_psa(pyrscc_scrubber_product
);
[total_hydrogen] =
calc_hydrogen(pyrscc_psa_product
);

[PEC_pyrolysis]=calc_cost_pyroly
sis(X);
[PEC_gasifier]=calc_cost_sccgasi
fier(pyr_input);
[PEC_filter]=calc_cost_filter(py
rscc_output);
[PEC_scrubber]=calc_cost_scrubbe
r(pyrscc_filter_product);
[PEC_psa]=calc_cost_psa(pyrscc_s
crubber_product);
[PEC_furnace]=calc_cost_furnance
(pyr_input);
[PEC_boiler]=calc_cost_boiler(st
eamflow);
[PEC] =
calc_PEC2(PEC_pyrolysis,PEC_gasi
fier,PEC_filter,PEC_scrubber,PEC
_psa,PEC_furnace,PEC_boiler);

[FCI] = calc_FCI(PEC);
[TPC] =
calc_TPC(FCI,X,steamflow);
[TCI] = calc_TCI(FCI);
[hydrogencost] =
calc_hydrogencost(TCI,TPC,total_
hydrogen);

end
```

Route with Constraints

```
function[c,ceq]=calc_hydrogencos
t_pyrscc_constraints(X)

[pyr_input] = calc_pyrolysis(X);
[pyrscc_output,steamflow] =
calc_scc(pyr_input);
[pyrscc_filter_product] =
calc_filter(pyrscc_output);
[pyrscc_scrubber_product] =
calc_scrubber(pyrscc_filter_prod
uct);
[pyrscc_psa_product] =
calc_psa(pyrscc_scrubber_product
);
[total_hydrogen] =
calc_hydrogen(pyrscc_psa_product
);

[PEC_pyrolysis]=calc_cost_pyroly
sis(X);
[PEC_gasifier]=calc_cost_sccgasi
fier(pyr_input);
[PEC_filter]=calc_cost_filter(py
rscc_output);
[PEC_scrubber]=calc_cost_scrubbe
r(pyrscc_filter_product);
[PEC_psa]=calc_cost_psa(pyrscc_s
crubber_product);
[PEC_furnace]=calc_cost_furnance
(pyr_input);
[PEC_boiler]=calc_cost_boiler(st
eamflow);
[PEC] =
calc_PEC2(PEC_pyrolysis,PEC_gasi
fier,PEC_filter,PEC_scrubber,PEC
_psa,PEC_furnace,PEC_boiler);

[FCI] = calc_FCI(PEC);
[TPC] =
calc_TPC(FCI,X,steamflow);
```

```
[TCI] = calc_TCI(FCI);
[hydrogencost] =
calc_hydrogencost(TCI,TPC,total_
hydrogen);

ceq=[];
c=2.3-hydrogencost;

end
```

Fast Pyrolysis Chamber

```
function [pyr_input] =
calc_pyrolysis(efb)
pyr_char=efb*0.251;
pyr_input=pyr_char;
end
```

Steam Gasification with Carbon Capture

```
function[output,steamflow] =
calc_scc(input)
steamflow=input*3;
product=input*3.54;
output=product;
end
```

Filter

```
function [filter_product] =
calc_filter(output)
filter_product=output*0.963;
end
```

Scrubber

```
function [scrubber_product] =
calc_scrubber(filter_product)
scrubber_product=filter_product*
0.247;
end
```

Pressure Swing Adsorption Column

```
function [psa_product] =
calc_psa(filter_product)
psa_product=filter_product*0.110
;
end
```

Amount of Hydrogen Produced

```
function [total_hydrogen] =
calc_hydrogen(psa_byproduct)
total_hydrogen=psa_byproduct;
end
```

Cost of Fast Pyrolysis Chamber

```
function
[pyrolysis_cost]=calc_cost_pyrol
ysis(flowrate)
pm=0.49096; % density of EFB
(g/m3)
F=flowrate; % flowrate at
gasifier
k=98.7;
x=0.251;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2; % SS
MS=1491.7;
pyrolysis_cost=(MS/280)*101.9*(D
r^1.066)*(Lr^0.82)*Fc;
end
```

Cost of Steam Gasification with Carbon Capture

```
function
[gasifier_cost]=calc_cost_sccgas
ifier(flowrate)
pm=0.49096;
F=flowrate;
k=98.7;
x=0.708;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
gasifier_cost=(MS/280)*101.9*(Dr
^1.066)*(Lr^0.82)*Fc;
end
```

Cost of Filter

```
function
[filter_cost]=calc_cost_filter(f
lowrate)
pm=0.49096;
F=flowrate;
k=98.7;
x=0.963;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
filter_cost=(MS/280)*101.9*(Dr^1
.066)*(Lr^0.82)*Fc;
end
```

Cost of Scrubber

```
function
[scrubber_cost]=calc_cost_scrubb
er(flowrate)
pm=0.49096; % density of EFB
(g/m3)
F=flowrate;
k=98.7;
x=0.138;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
scrubber_cost=(MS/280)*101.9*(Dr
^1.066)*(Lr^0.82)*Fc;
end
```

Cost of Pressure Swing Adsorption

```
function
[scrubber_cost]=calc_cost_psa(fl
owrate)
pm=0.49096; % density of EFB
(g/m3)
F=flowrate;
k=98.7;
x=0.110;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
scrubber_cost=(MS/280)*101.9*(Dr
^1.066)*(Lr^0.82)*Fc;
end
```

Cost of Furnace

```
function
[furnance_cost]=calc_cost_furnan
ce(QeeQ)
QeeQ=100;
Q=QeeQ*9.47*10^-10; % energy req
for gasification process QeeQ is
in J/hr and converted to Mbtu/hr
pm=0.49096; % density of EFB
(g/m3)
Fc=1; % based on assumption that
stainless steel materilas
MS=1491.70; %from Chemical
Engineering magazine
furnance_cost=(MS/280)*(5.52*10^
3)*(Q^0.85)*Fc;
end
```

Cost of Boiler

```
function
[boiler_cost]=calc_cost_boiler(s
teamflow)
ST=steamflow;
MD=1000;
boiler_cost=(3.28*10^5)*(ST/MD)^
0.81;
end
```

Purchased Equipment Cost

```
function [PEC] =
calc_PEC2(PEC_pretreatment,PEC_g
asifier,PEC_filter,PEC_scrubber,
PEC_psa,PEC_furnace,PEC_boiler)
PEC=PEC_pretreatment+PEC_gasifie
r+PEC_filter+PEC_scrubber+PEC_ps
a+PEC_furnace+PEC_boiler;
end
```

Fixed Capital Investment

```
function [FCI] = calc_FCI(PEC)
DC=3.778*PEC;
IC=0.4165*PEC;
FCI=DC+IC;
end
```

Total Production Cost

```
function [TPC] =
calc_TPC(FCI,efb,steamflow)
rawcost=efb*0.015; % Assuming
efb in kg/hr and efb costs USD
0.015/kg
utility=12.90; % USD 12.90/kg.
Taken from P. Lv et al.
steamcost=steamflow*0.002; % USD
0.002/kg. Taken from Hamada
Boiler Malaysia, 2008
catalystcost=efb*7.8279; % USD
7.8279/kg.  Taken from P. Lv et
al.
sorbentcost=efb*0.098; % USD
0.098/kg. Taken from iCheme
Website, 2002
OL=0.15*FCI;
supervision=0.15*OL;
repair=0.05*FCI;
TDPC=rawcost+utility+steamcost+c
atalystcost+sorbentcost+OL+super
vision+repair;
TPC=TDPC;
end
```

Total Capital Investment

```
function [TCI] = calc_TCI(FCI)
WC=0.2*FCI;
TCI=FCI+WC;
end
```

Cost of Hydrogen Produced

```
function [hydrogencost] =
calc_hydrogencost(TCI,TPC,total_
hydrogen)
TC=TCI+TPC;
hydrogencost=TC/total_hydrogen;
end
```

Optimization

```
% define the initial guess
independent variables for
optimization
X0=1;
% define the lower bounds for
independent variables
LB=[];
% define the upper bounds for
independent variables
UB=[];
% define the coefficients for
the linear inequality
constraints
A = [];
B = [];
% define the coefficients for
the linear equality constraints
Aeq = [];
Beq = [];
% define the options for the
optimization solver
options =
optimset('Algorithm','interior-
point','Display',
'iter','MaxFunEvals',1e6,'MaxIte
r',1e6, ...
    'TolFun',1e-
6,'TolConSQP',1e-6,'TolX',1e-
6,'FunValCheck','on');
% solving the optimization
problem
[X,FVAL,EXITFLAG,OUTPUT,LAMBDA,G
RAD,HESSIAN]=fmincon(@calc_hydro
gencost_pyrscc,X0,A,B,Aeq,Beq,LB
,UB,@calc_hydrogencost_pyrscc_co
nstraints,options);
```

Route F: Pretreatment–Fast Pyrolysis, Gasification Agent–Steam and Oxygen with Carbon Capture

Route

```
function[hydrogencost]=calc_hydr
ogencost_pyrsocc(X)

[pyr_input] = calc_pyrolysis(X);
[pyrsocc_output,steamflow] =
calc_socc(pyr_input);
[pyrsocc_filter_product] =
calc_filter(pyrsocc_output);
```

```
[pyrsocc_scrubber_product] =
calc_scrubber(pyrsocc_filter_pro
duct);
[pyrsocc_psa_product] =
calc_psa(pyrsocc_scrubber_produc
t);
[total_hydrogen] =
calc_hydrogen(pyrsocc_psa_produc
t);

[PEC_pyrolysis]=calc_cost_pyroly
sis(X);
[PEC_gasifier]=calc_cost_soccgas
ifier(pyr_input);
[PEC_filter]=calc_cost_filter(py
rsocc_output);
[PEC_scrubber]=calc_cost_scrubbe
r(pyrsocc_filter_product);
[PEC_psa]=calc_cost_psa(pyrsocc_
scrubber_product);
[PEC_furnace]=calc_cost_furnance
(pyr_input);
[PEC_boiler]=calc_cost_boiler(st
eamflow);
[PEC] =
calc_PEC2(PEC_pyrolysis,PEC_gasi
fier,PEC_filter,PEC_scrubber,PEC
_psa,PEC_furnace,PEC_boiler);

[FCI] = calc_FCI(PEC);
[TPC] =
calc_TPC(FCI,X,steamflow);
[TCI] = calc_TCI(FCI);
[hydrogencost] =
calc_hydrogencost(TCI,TPC,total_
hydrogen);

end
```

Route with Constraints

```
function[c,ceq]=calc_hydrogencos
t_pyrsocc_constraints(X)

[pyr_input] = calc_pyrolysis(X);
[pyrsocc_output,steamflow] =
calc_socc(pyr_input);
[pyrsocc_filter_product] =
calc_filter(pyrsocc_output);
[pyrsocc_scrubber_product] =
calc_scrubber(pyrsocc_filter_pro
duct);
[pyrsocc_psa_product] =
calc_psa(pyrsocc_scrubber_produc
t);
[total_hydrogen] =
calc_hydrogen(pyrsocc_psa_produc
t);

[PEC_pyrolysis]=calc_cost_pyroly
sis(X);
[PEC_gasifier]=calc_cost_soccgas
ifier(pyr_input);
[PEC_filter]=calc_cost_filter(py
rsocc_output);
[PEC_scrubber]=calc_cost_scrubbe
r(pyrsocc_filter_product);
[PEC_psa]=calc_cost_psa(pyrsocc_
scrubber_product);
[PEC_furnace]=calc_cost_furnance
(pyr_input);
[PEC_boiler]=calc_cost_boiler(st
eamflow);
[PEC] =
calc_PEC2(PEC_pyrolysis,PEC_gasi
fier,PEC_filter,PEC_scrubber,PEC
_psa,PEC_furnace,PEC_boiler);

[FCI] = calc_FCI(PEC);
[TPC] =
calc_TPC(FCI,X,steamflow);
[TCI] = calc_TCI(FCI);
[hydrogencost] =
calc_hydrogencost(TCI,TPC,total_
hydrogen);

ceq=[];
c=2.3-hydrogencost;

end
```

Fast Pyrolysis Chamber

```
function [pyr_input] =
calc_pyrolysis(efb)
pyr_char=efb*0.251;
pyr_input=pyr_char;
end
```

Steam with Oxygen Gasification with Carbon Capture

```
function [output,socc_steamflow]
= calc_socc(input)
socc_steamflow=input*4.342;
socc_product=input*9.708;
output=socc_product;
end
```

Filter

```
function [filter_product] =
calc_filter(output)
filter_product=output*0.963;
end
```

Scrubber

```
function [scrubber_product] =
calc_scrubber(filter_product)
scrubber_product=filter_product*
0.247;
end
```

Pressure Swing Adsorption Column

```
function [psa_product] =
calc_psa(filter_product)
psa_product=filter_product*0.110
;
end
```

Amount of Hydrogen Produced

```
function [total_hydrogen] =
calc_hydrogen(psa_byproduct)
total_hydrogen=psa_byproduct;
end
```

Cost of Fast Pyrolysis Chamber

```
function
[pyrolysis_cost]=calc_cost_pyrol
ysis(flowrate)
pm=0.49096; % density of EFB
(g/m3)
F=flowrate; % flowrate at
gasifier
k=98.7;
x=0.251;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2; % SS
MS=1491.7;
pyrolysis_cost=(MS/280)*101.9*(D
r^1.066)*(Lr^0.82)*Fc;
end
```

Cost of Steam with Oxygen Gasification with Carbon Capture

```
function
[gasifier_cost]=calc_cost_soccga
sifier(flowrate)
pm=0.49096;
F=flowrate;
k=98.7;
x=0.761;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
gasifier_cost=(MS/280)*101.9*(Dr
^1.066)*(Lr^0.82)*Fc;
end
```

Cost of Filter

```
function
[filter_cost]=calc_cost_filter(f
lowrate)
pm=0.49096;
F=flowrate;
k=98.7;
x=0.963;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=((0.66*3.142*V)+eps)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
filter_cost=(MS/280)*101.9*(Dr^1
.066)*(Lr^0.82)*Fc;
end
```

Cost of Scrubber

```
function
[scrubber_cost]=calc_cost_scrubb
er(flowrate)
pm=0.49096; % density of EFB
(g/m3)
F=flowrate;
k=98.7;
```

```
x=0.138;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
scrubber_cost=(MS/280)*101.9*(Dr
^1.066)*(Lr^0.82)*Fc;
end
```

Cost of Pressure Swing Adsorption

```
function
[scrubber_cost]=calc_cost_psa(fl
owrate)
pm=0.49096; % density of EFB
(g/m3)
F=flowrate;
k=98.7;
x=0.110;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
scrubber_cost=(MS/280)*101.9*(Dr
^1.066)*(Lr^0.82)*Fc;
end
```

Cost of Furnace

```
function
[furnance_cost]=calc_cost_furnan
ce(QeeQ)
QeeQ=100;
Q=QeeQ*9.47*10^-10; % energy req
for gasification process QeeQ is
in J/hr and converted to Mbtu/hr
pm=0.49096; % density of EFB
(g/m3)
Fc=1; % based on assumption that
stainless steel materilas
MS=1491.70; %from Chemical
Engineering magazine
furnance_cost=(MS/280)*(5.52*10^
3)*(Q^0.85)*Fc;
end
```

Cost of Boiler

```
function
[boiler_cost]=calc_cost_boiler(s
teamflow)
ST=steamflow;
MD=1000;
boiler_cost=(3.28*10^5)*(ST/MD)^
0.81;
end
```

Purchased Equipment Cost

```
function [PEC] =
calc_PEC2(PEC_pretreatment,PEC_g
asifier,PEC_filter,PEC_scrubber,
PEC_psa,PEC_furnace,PEC_boiler)
PEC=PEC_pretreatment+PEC_gasifie
r+PEC_filter+PEC_scrubber+PEC_ps
a+PEC_furnace+PEC_boiler;
end
```

Fixed Capital Investment

```
function [FCI] = calc_FCI(PEC)
DC=3.778*PEC;
IC=0.4165*PEC;
FCI=DC+IC;
end
```

Total Production Cost

```
function [TPC] =
calc_TPC(FCI,efb,steamflow)
rawcost=efb*0.015; % Assuming
efb in kg/hr and efb costs USD
0.015/kg
utility=12.90; % USD 12.90/kg.
Taken from P. Lv et al.
steamcost=steamflow*0.002; % USD
0.002/kg. Taken from Hamada
Boiler Malaysia, 2008
catalystcost=efb*7.8279; % USD
7.8279/kg.  Taken from P. Lv et
al.
sorbentcost=efb*0.098; % USD
0.098/kg. Taken from iCheme
Website, 2002
OL=0.15*FCI;
supervision=0.15*OL;
repair=0.05*FCI;
TDPC=rawcost+utility+steamcost+c
atalystcost+sorbentcost+OL+super
vision+repair;
```

```
TPC=TDPC;
end
```

Total Capital Investment

```
function [TCI] = calc_TCI(FCI)
WC=0.2*FCI;
TCI=FCI+WC;
end
```

Cost of Hydrogen Produced

```
function [hydrogencost] =
calc_hydrogencost(TCI,TPC,total_
hydrogen)
TC=TCI+TPC;
hydrogencost=TC/total_hydrogen;
end
```

Optimization

```
% define the initial guess
independent variables for
optimization
X0=1;
% define the lower bounds for
independent variables
LB=[];
% define the upper bounds for
independent variables
UB=[];
% define the coefficients for
the linear inequality
constraints
A = [];
B = [];
% define the coefficients for
the linear equality constraints
Aeq = [];
Beq = [];
% define the options for the
optimization solver
options =
optimset('Algorithm','active-
set','Display',
'iter','MaxFunEvals',1e6,'MaxIte
r',1e6, ...
    'TolFun',1e-
6,'TolConSQP',1e-6,'TolX',1e-
6,'FunValCheck','on');
% solving the optimization
problem
[X,FVAL,EXITFLAG,OUTPUT,LAMBDA,G
RAD,HESSIAN]=fmincon(@calc_hydro
gencost_pyrsocc,X0,A,B,Aeq,Beq,L
B,UB,@calc_hydrogencost_pyrsocc_
constraints,options);
```

Route G: Pretreatment–Drying with Superheated Steam, Gasification Agent–Air

Route

```
function[hydrogencost]=calc_hydr
ogencost_dryair(X)

[dry_input,steamflow] =
calc_drying1(X);
[dryair_output] =
calc_air2(dry_input);
[dryair_filter_product] =
calc_filter2(dryair_output);
[dryair_scrubber_product] =
calc_scrubber2(dryair_filter_pro
duct);
[dryair_psa_product] =
calc_psa2(dryair_scrubber_produc
t);
[total_hydrogen] =
calc_hydrogen2(dryair_psa_produc
t);

[PEC_dryer]=calc_cost_dryer(X);
[PEC_gasifier]=calc_cost_airgasi
fier(dry_input);
[PEC_filter]=calc_cost_filter(dr
yair_output);
[PEC_scrubber]=calc_cost_scrubbe
r(dryair_filter_product);
[PEC_psa]=calc_cost_psa(dryair_s
crubber_product);
[PEC_furnace]=calc_cost_furnance
(dry_input);
[PEC_boiler]=calc_cost_boiler(st
eamflow);
[PEC] =
calc_PEC2(PEC_dryer,PEC_gasifier
,PEC_filter,PEC_scrubber,PEC_psa
,PEC_furnace,PEC_boiler);

[FCI] = calc_FCI(PEC);
[TPC] =
calc_TPC(FCI,X,steamflow);
[TCI] = calc_TCI(FCI);
[hydrogencost] =
calc_hydrogencost(TCI,TPC,total_
hydrogen);
```

```
end
```

Route with Constraints

```
function[c,ceq]=calc_hydrogencos
t_dryair_constraints(X)

[dry_input,steamflow] =
calc_drying1(X);
[dryair_output] =
calc_air2(dry_input);
[dryair_filter_product] =
calc_filter2(dryair_output);
[dryair_scrubber_product] =
calc_scrubber2(dryair_filter_pro
duct);
[dryair_psa_product] =
calc_psa2(dryair_scrubber_produc
t);
[total_hydrogen] =
calc_hydrogen2(dryair_psa_produc
t);

[PEC_dryer]=calc_cost_dryer(X);
[PEC_gasifier]=calc_cost_airgasi
fier(dry_input);
[PEC_filter]=calc_cost_filter(dr
yair_output);
[PEC_scrubber]=calc_cost_scrubbe
r(dryair_filter_product);
[PEC_psa]=calc_cost_psa(dryair_s
crubber_product);
[PEC_furnace]=calc_cost_furnance
(dry_input);
[PEC_boiler]=calc_cost_boiler(st
eamflow);
[PEC] =
calc_PEC2(PEC_dryer,PEC_gasifier
,PEC_filter,PEC_scrubber,PEC_psa
,PEC_furnace,PEC_boiler);

[FCI] = calc_FCI(PEC);
[TPC] =
calc_TPC(FCI,X,steamflow);
[TCI] = calc_TCI(FCI);
[hydrogencost] =
calc_hydrogencost(TCI,TPC,total_
hydrogen);

ceq=[];
c=2.3-hydrogencost;

end
```

Drying Chamber

```
function[dry_input,steamflow] =
calc_drying1(efb)
dry_product=efb*0.973;
dry_input=dry_product;
steamflow=efb*2.05;
end
```

Air Gasification

```
function[dryair_output] =
calc_air2(dry_input)
dryair_product=dry_input*0.1;
dryair_output=dryair_product;
end
```

Filter

```
function[dryair_filter_product]
= calc_filter2(dryair_output)
dryair_filter_product=dryair_out
put*0.963;
end
```

Scrubber

```
function[dryair_scrubber_product
] =
calc_scrubber2(dryair_filter_pro
duct)
dryair_scrubber_product=dryair_f
ilter_product*0.247;
end
```

Pressure Swing Adsorption Column

```
function[dryair_psa_product] =
calc_psa2(dryair_scrubber_produc
t)
dryair_psa_product=dryair_scrubb
er_product*0.110;
end
```

Amount of Hydrogen Produced

```
function[total_hydrogen] =
calc_hydrogen2(dryair_psa_produc
t)
total_hydrogen=dryair_psa_produc
t;
```

```
end
```

Cost of Drying Chamber

```
function
[dryer_cost]=calc_cost_dryer(flo
wrate)
pm=0.49096; % density of EFB
(g/m3)
F=flowrate; % flowrate at
gasifier
k=98.7;
x=0.973; % based on literature:
HASIBUAN & WAN DAUD (2004)
a=F*log(1/(1-x));
b=k*pm;
V=a/b; %volume of gasifier
% L/D =6 (assumed based on
douglas)page 507
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2; % SS
MS=1491.7; %from Chemical
Engineering magazine
dryer_cost=(MS/280)*101.9*(Dr^1.
066)*(Lr^0.82)*Fc;
end
```

Cost of Air Gasification

```
function
[gasifier_cost]=calc_cost_airgas
ifier(flowrate)
pm=0.49096;
F=flowrate;
k=98.7;
x=0.0413;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
gasifier_cost=(MS/280)*101.9*(Dr
^1.066)*(Lr^0.82)*Fc;
end
```

Cost of Filter

```
function
[filter_cost]=calc_cost_filter(f
lowrate)
pm=0.49096;
F=flowrate;
k=98.7;
x=0.963;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
filter_cost=(MS/280)*101.9*(Dr^1
.066)*(Lr^0.82)*Fc;
end
```

Cost of Scrubber

```
function
[scrubber_cost]=calc_cost_scrubb
er(flowrate)
pm=0.49096; % density of EFB
(g/m3)
F=flowrate;
k=98.7;
x=0.138;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
scrubber_cost=(MS/280)*101.9*(Dr
^1.066)*(Lr^0.82)*Fc;
end
```

Cost of Pressure Swing Adsorption

```
function
[scrubber_cost]=calc_cost_psa(fl
owrate)
pm=0.49096; % density of EFB
(g/m3)
F=flowrate;
k=98.7;
```

```
x=0.110;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
scrubber_cost=(MS/280)*101.9*(Dr
^1.066)*(Lr^0.82)*Fc;
end
```

Cost of Furnace

```
function
[furnance_cost]=calc_cost_furnan
ce(QeeQ)
QeeQ=100;
Q=QeeQ*9.47*10^-10; % energy req
for gasification process QeeQ is
in J/hr and converted to Mbtu/hr
pm=0.49096; % density of EFB
(g/m3)
Fc=1; % based on assumption that
stainless steel materilas
MS=1491.70; %from Chemical
Engineering magazine
furnance_cost=(MS/280)*(5.52*10^
3)*(Q^0.85)*Fc;
end
```

Cost of Boiler

```
function
[boiler_cost]=calc_cost_boiler(s
teamflow)
ST=steamflow;
MD=1000;
boiler_cost=(3.28*10^5)*(ST/MD)^
0.81;
end
```

Purchased Equipment Cost

```
function [PEC] =
calc_PEC2(PEC_pretreatment,PEC_g
asifier,PEC_filter,PEC_scrubber,
PEC_psa,PEC_furnace,PEC_boiler)
PEC=PEC_pretreatment+PEC_gasifie
r+PEC_filter+PEC_scrubber+PEC_ps
a+PEC_furnace+PEC_boiler;
end
```

Fixed Capital Investment

```
function [FCI] = calc_FCI(PEC)
DC=3.778*PEC;
IC=0.4165*PEC;
FCI=DC+IC;
end
```

Total Production Cost

```
function [TPC] =
calc_TPC(FCI,efb,steamflow)
rawcost=efb*0.015; % Assuming
efb in kg/hr and efb costs USD
0.015/kg
utility=12.90; % USD 12.90/kg.
Taken from P. Lv et al.
steamcost=steamflow*0.002; % USD
0.002/kg. Taken from Hamada
Boiler Malaysia, 2008
catalystcost=efb*7.8279; % USD
7.8279/kg.  Taken from P. Lv et
al.
sorbentcost=efb*0.098; % USD
0.098/kg. Taken from iCheme
Website, 2002
OL=0.15*FCI;
supervision=0.15*OL;
repair=0.05*FCI;
TDPC=rawcost+utility+steamcost+c
atalystcost+sorbentcost+OL+super
vision+repair;
TPC=TDPC;
end
```

Total Capital Investment

```
function [TCI] = calc_TCI(FCI)
WC=0.2*FCI;
TCI=FCI+WC;
end
```

Cost of Hydrogen Produced

```
function [hydrogencost] =
calc_hydrogencost(TCI,TPC,total_
hydrogen)
TC=TCI+TPC;
hydrogencost=TC/total_hydrogen;
end
```

Optimization

```
% define the initial guess
independent variables for
optimization
%
[k1,E1,k2,E2,k3,E3,k4,E4,k5,E5,k
6,E6]
X0=1;
% define the lower bounds for
independent variables
LB=[];
% define the upper bounds for
independent variables
UB=[];
% define the coefficients for
the linear inequality
constraints
A = [];
B = [];
% define the coefficients for
the linear equality constraints
Aeq = [];
Beq = [];
% define the options for the
optimization solver
options =
optimset('Algorithm','active-
set','Display','iter','MaxFunEva
ls',1e6,'MaxIter',1e6, ...
    'TolFun',1e-
6,'TolConSQP',1e-6,'TolX',1e-
6,'FunValCheck','on');
% solving the optimization
problem
[X,FVAL,EXITFLAG,OUTPUT,LAMBDA,G
RAD,HESSIAN]=fmincon(@calc_hydro
gencost_dryair,X0,A,B,Aeq,Beq,LB
,UB,@calc_hydrogencost_dryair_co
nstraints,options);
```

<u>Route H</u>: Pretreatment–Drying with Superheated Steam, Gasification Agent–Steam with Carbon Capture

Route

```
function[hydrogencost]=calc_hydr
ogencost_dryscc(X)

[dry_input,steamflow1] =
calc_drying1(X);
[dryscc_output,steamflow2] =
calc_scc(dry_input);
[dryscc_filter_product] =
calc_filter(dryscc_output);
[dryscc_scrubber_product] =
calc_scrubber(dryscc_filter_prod
uct);
[dryscc_psa_product] =
calc_psa(dryscc_scrubber_product
);
[total_hydrogen] =
calc_hydrogen(dryscc_psa_product
);

[PEC_dryer]=calc_cost_dryer(X);
[PEC_gasifier]=calc_cost_sccgasi
fier(dry_input);
[PEC_filter]=calc_cost_filter(dr
yscc_output);
[PEC_scrubber]=calc_cost_scrubbe
r(dryscc_filter_product);
[PEC_psa]=calc_cost_psa(dryscc_s
crubber_product);
[PEC_furnace]=calc_cost_furnance
(dry_input);
[PEC_boiler]=calc_cost_boiler(st
eamflow1,steamflow2);
[PEC] =
calc_PEC2(PEC_dryer,PEC_gasifier
,PEC_filter,PEC_scrubber,PEC_psa
,PEC_furnace,PEC_boiler);

[FCI] = calc_FCI(PEC);
[TPC] =
calc_TPC(FCI,X,steamflow1,steamf
low2);
[TCI] = calc_TCI(FCI);
[hydrogencost] =
calc_hydrogencost(TCI,TPC,total_
hydrogen);

end
```

Route with Constraints

```
function[c,ceq]=calc_hydrogencos
t_dryscc_constraints(X)

[dry_input,steamflow1] =
calc_drying1(X);
[dryscc_output,steamflow2] =
calc_scc(dry_input);
[dryscc_filter_product] =
calc_filter(dryscc_output);
```

```
[dryscc_scrubber_product] =
calc_scrubber(dryscc_filter_prod
uct);
[dryscc_psa_product] =
calc_psa(dryscc_scrubber_product
);
[total_hydrogen] =
calc_hydrogen(dryscc_psa_product
);

[PEC_dryer]=calc_cost_dryer(X);
[PEC_gasifier]=calc_cost_sccgasi
fier(dry_input);
[PEC_filter]=calc_cost_filter(dr
yscc_output);
[PEC_scrubber]=calc_cost_scrubbe
r(dryscc_filter_product);
[PEC_psa]=calc_cost_psa(dryscc_s
crubber_product);
[PEC_furnace]=calc_cost_furnance
(dry_input);
[PEC_boiler]=calc_cost_boiler(st
eamflow1,steamflow2);
[PEC] =
calc_PEC2(PEC_dryer,PEC_gasifier
,PEC_filter,PEC_scrubber,PEC_psa
,PEC_furnace,PEC_boiler);

[FCI] = calc_FCI(PEC);
[TPC] =
calc_TPC(FCI,X,steamflow1,steamf
low2);
[TCI] = calc_TCI(FCI);
[hydrogencost] =
calc_hydrogencost(TCI,TPC,total_
hydrogen);

ceq=[];
c=2.3-hydrogencost;

end
```

Drying Chamber

```
function[dry_input,steamflow] =
calc_drying1(efb)
dry_product=efb*0.973;
dry_input=dry_product;
steamflow=efb*2.05;
end
```

Steam Gasification with Carbon Capture

```
function[output,steamflow] =
calc_scc(input)
steamflow=input*3;
product=input*3.54;
output=product;
end
```

Filter

```
function [filter_product] =
calc_filter(output)
filter_product=output*0.963;
end
```

Scrubber

```
function [scrubber_product] =
calc_scrubber(filter_product)
scrubber_product=filter_product*
0.247;
end
```

Pressure Swing Adsorption Column

```
function [psa_product] =
calc_psa(filter_product)
psa_product=filter_product*0.110
;
end
```

Amount of Hydrogen Produced

```
function [total_hydrogen] =
calc_hydrogen(psa_byproduct)
total_hydrogen=psa_byproduct;
end
```

Cost of Drying Chamber

```
function
[dryer_cost]=calc_cost_dryer(flo
wrate)
pm=0.49096; % density of EFB
(g/m3)
F=flowrate; % flowrate at
gasifier
k=98.7;
x=0.973; % based on literature:
HASIBUAN & WAN DAUD (2004)
a=F*log(1/(1-x));
b=k*pm;
V=a/b; %volume of gasifier
% L/D =6 (assumed based on
douglas)page 507
L_D=4; %Lr/Dr=4
```

```
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2; % SS
MS=1491.7; %from Chemical
Engineering magazine
dryer_cost=(MS/280)*101.9*(Dr^1.
066)*(Lr^0.82)*Fc;
end
```

Cost of Steam Gasification with Carbon Capture

```
function
[gasifier_cost]=calc_cost_sccgas
ifier(flowrate)
pm=0.49096;
F=flowrate;
k=98.7;
x=0.708;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
gasifier_cost=(MS/280)*101.9*(Dr
^1.066)*(Lr^0.82)*Fc;
end
```

Cost of Filter

```
function
[filter_cost]=calc_cost_filter(f
lowrate)
pm=0.49096;
F=flowrate;
k=98.7;
x=0.963;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
filter_cost=(MS/280)*101.9*(Dr^1
.066)*(Lr^0.82)*Fc;
end
```

Cost of Scrubber

```
function
[scrubber_cost]=calc_cost_scrubb
er(flowrate)
pm=0.49096; % density of EFB
(g/m3)
F=flowrate;
k=98.7;
x=0.138;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
scrubber_cost=(MS/280)*101.9*(Dr
^1.066)*(Lr^0.82)*Fc;
end
```

Cost of Pressure Swing Adsorption

```
function
[scrubber_cost]=calc_cost_psa(fl
owrate)
pm=0.49096; % density of EFB
(g/m3)
F=flowrate;
k=98.7;
x=0.110;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
scrubber_cost=(MS/280)*101.9*(Dr
^1.066)*(Lr^0.82)*Fc;
end
```

Cost of Furnace

```
function
[furnance_cost]=calc_cost_furnan
ce(QeeQ)
QeeQ=100;
Q=QeeQ*9.47*10^-10; % energy req
for gasification process QeeQ is
in J/hr and converted to Mbtu/hr
```

```
pm=0.49096; % density of EFB
(g/m3)
Fc=1; % based on assumption that
stainless steel materilas
MS=1491.70; %from Chemical
Engineering magazine
furnance_cost=(MS/280)*(5.52*10^
3)*(Q^0.85)*Fc;
end
```

Cost of Boiler

```
function
[boiler_cost]=calc_cost_boiler(s
teamflow1,steamflow2)
ST=steamflow1+steamflow2;
MD=1000;
boiler_cost=(3.28*10^5)*(ST/MD)^
0.81;
end
```

Purchased Equipment Cost

```
function [PEC] =
calc_PEC2(PEC_pretreatment,PEC_g
asifier,PEC_filter,PEC_scrubber,
PEC_psa,PEC_furnace,PEC_boiler)
PEC=PEC_pretreatment+PEC_gasifie
r+PEC_filter+PEC_scrubber+PEC_ps
a+PEC_furnace+PEC_boiler;
end
```

Fixed Capital Investment

```
function [FCI] = calc_FCI(PEC)
DC=3.778*PEC;
IC=0.4165*PEC;
FCI=DC+IC;
end
```

Total Production Cost

```
function [TPC] =
calc_TPC(FCI,efb,steamflow1,stea
mflow2)
rawcost=efb*0.015; % Assuming
efb in kg/hr and efb costs USD
0.015/kg
utility=12.90; % USD 12.90/kg.
Taken from P. Lv et al.
steamcost=(steamflow1+steamflow2
)*0.002; % USD 0.002/kg. Taken
from Hamada Boiler Malaysia,
2008
catalystcost=efb*7.8279; % USD
7.8279/kg.  Taken from P. Lv et
al.
sorbentcost=efb*0.098; % USD
0.098/kg. Taken from iCheme
Website, 2002
OL=0.15*FCI;
supervision=0.15*OL;
repair=0.05*FCI;
TDPC=rawcost+utility+steamcost+c
atalystcost+sorbentcost+OL+super
vision+repair;
TPC=TDPC;
end
```

Total Capital Investment

```
function [TCI] = calc_TCI(FCI)
WC=0.2*FCI;
TCI=FCI+WC;
end
```

Cost of Hydrogen Produced

```
function [hydrogencost] =
calc_hydrogencost(TCI,TPC,total_
hydrogen)
TC=TCI+TPC;
hydrogencost=TC/total_hydrogen;
end
```

Optimization

```
% define the initial guess
independent variables for
optimization
X0=1;
% define the lower bounds for
independent variables
LB=[];
% define the upper bounds for
independent variables
UB=[];
% define the coefficients for
the linear inequality
constraints
A = [];
B = [];
% define the coefficients for
the linear equality constraints
Aeq = [];
Beq = [];
% define the options for the
optimization solver
```

```
options =
optimset('Algorithm','interior-point','Display',
'iter','MaxFunEvals',1e6,'MaxIter',1e6, ...
    'TolFun',1e-6,'TolConSQP',1e-6,'TolX',1e-6,'FunValCheck','on');
% solving the optimization problem
[X,FVAL,EXITFLAG,OUTPUT,LAMBDA,GRAD,HESSIAN]=fmincon(@calc_hydrogencost_dryscc,X0,A,B,Aeq,Beq,LB,UB,@calc_hydrogencost_dryscc_constraints,options);
```

Route I: **Pretreatment–Drying with Superheated Steam, Gasification Agent–Steam and Oxygen with Carbon Capture**

Route

```
function[hydrogencost]=calc_hydrogencost_drysocc(X)

[dry_input,steamflow1] =
calc_drying1(X);
[drysocc_output,steamflow2] =
calc_socc(dry_input);
[drysocc_filter_product] =
calc_filter(drysocc_output);
[drysocc_scrubber_product] =
calc_scrubber(drysocc_filter_product);
[drysocc_psa_product] =
calc_psa(drysocc_scrubber_product);
[total_hydrogen] =
calc_hydrogen(drysocc_psa_product);

[PEC_dryer]=calc_cost_dryer(X);
[PEC_gasifier]=calc_cost_soccgasifier(dry_input);
[PEC_filter]=calc_cost_filter(drysocc_output);
[PEC_scrubber]=calc_cost_scrubber(drysocc_filter_product);
[PEC_psa]=calc_cost_psa(drysocc_scrubber_product);
[PEC_furnace]=calc_cost_furnance(dry_input);
[PEC_boiler]=calc_cost_boiler(steamflow1,steamflow2);
[PEC] =
calc_PEC2(PEC_dryer,PEC_gasifier,PEC_filter,PEC_scrubber,PEC_psa,PEC_furnace,PEC_boiler);

[FCI] = calc_FCI(PEC);
[TPC] =
calc_TPC(FCI,X,steamflow1,steamflow2);
[TCI] = calc_TCI(FCI);
[hydrogencost] =
calc_hydrogencost(TCI,TPC,total_hydrogen);

end
```

Route with Constraints

```
function[c,ceq]=calc_hydrogencost_drysocc_constraints(X)

[dry_input,steamflow1] =
calc_drying1(X);
[drysocc_output,steamflow2] =
calc_socc(dry_input);
[drysocc_filter_product] =
calc_filter(drysocc_output);
[drysocc_scrubber_product] =
calc_scrubber(drysocc_filter_product);
[drysocc_psa_product] =
calc_psa(drysocc_scrubber_product);
[total_hydrogen] =
calc_hydrogen(drysocc_psa_product);

[PEC_dryer]=calc_cost_dryer(X);
[PEC_gasifier]=calc_cost_soccgasifier(dry_input);
[PEC_filter]=calc_cost_filter(drysocc_output);
[PEC_scrubber]=calc_cost_scrubber(drysocc_filter_product);
[PEC_psa]=calc_cost_psa(drysocc_scrubber_product);
[PEC_furnace]=calc_cost_furnance(dry_input);
[PEC_boiler]=calc_cost_boiler(steamflow1,steamflow2);
```

```
[PEC] =
calc_PEC2(PEC_dryer,PEC_gasifier
,PEC_filter,PEC_scrubber,PEC_psa
,PEC_furnace,PEC_boiler);

[FCI] = calc_FCI(PEC);
[TPC] =
calc_TPC(FCI,X,steamflow1,steamf
low2);
[TCI] = calc_TCI(FCI);
[hydrogencost] =
calc_hydrogencost(TCI,TPC,total_
hydrogen);

ceq=[];
c=2.3-hydrogencost;

end
```

Drying Chamber

```
function[dry_input,steamflow] =
calc_drying1(efb)
dry_product=efb*0.973;
dry_input=dry_product;
steamflow=efb*2.05;
end
```

Steam with Oxygen Gasification with Carbon Capture

```
function [output,socc_steamflow]
= calc_socc(input)
socc_steamflow=input*4.342;
socc_product=input*9.708;
output=socc_product;
end
```

Filter

```
function [filter_product] =
calc_filter(output)
filter_product=output*0.963;
end
```

Scrubber

```
function [scrubber_product] =
calc_scrubber(filter_product)
scrubber_product=filter_product*
0.247;
end
```

Pressure Swing Adsorption Column

```
function [psa_product] =
calc_psa(filter_product)
psa_product=filter_product*0.110
;
end
```

Amount of Hydrogen Produced

```
function [total_hydrogen] =
calc_hydrogen(psa_byproduct)
total_hydrogen=psa_byproduct;
end
```

Cost of DryingChamber

```
function
[dryer_cost]=calc_cost_dryer(flo
wrate)
pm=0.49096; % density of EFB
(g/m3)
F=flowrate; % flowrate at
gasifier
k=98.7;
x=0.973; % based on literature:
HASIBUAN & WAN DAUD (2004)
a=F*log(1/(1-x));
b=k*pm;
V=a/b; %volume of gasifier
% L/D =6 (assumed based on
douglas)page 507
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2; % SS
MS=1491.7; %from Chemical
Engineering magazine
dryer_cost=(MS/280)*101.9*(Dr^1.
066)*(Lr^0.82)*Fc;
end
```

Cost of Steam with Oxygen Gasification with Carbon Capture

```
function
[gasifier_cost]=calc_cost_soccga
sifier(flowrate)
pm=0.49096;
F=flowrate;
k=98.7;
x=0.761;
```

```
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
gasifier_cost=(MS/280)*101.9*(Dr
^1.066)*(Lr^0.82)*Fc;
end
```

Cost of Filter

```
function
[filter_cost]=calc_cost_filter(f
lowrate)
pm=0.49096;
F=flowrate;
k=98.7;
x=0.963;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
filter_cost=(MS/280)*101.9*(Dr^1
.066)*(Lr^0.82)*Fc;
end
```

Cost of Scrubber

```
function
[scrubber_cost]=calc_cost_scrubb
er(flowrate)
pm=0.49096; % density of EFB
(g/m3)
F=flowrate;
k=98.7;
x=0.138;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
scrubber_cost=(MS/280)*101.9*(Dr
^1.066)*(Lr^0.82)*Fc;
end
```

Cost of Pressure Swing Adsorption

```
function
[scrubber_cost]=calc_cost_psa(fl
owrate)
pm=0.49096; % density of EFB
(g/m3)
F=flowrate;
k=98.7;
x=0.110;
a=F*log(1/(1-x));
b=k*pm;
V=a/b;
L_D=4; %Lr/Dr=4
D=(0.66*3.142*V)^0.33;
Dr=D/0.4;
Lr=(L_D*Dr)/0.4;
Fc=1.2;
MS=1491.7;
scrubber_cost=(MS/280)*101.9*(Dr
^1.066)*(Lr^0.82)*Fc;
end
```

Cost of Furnace

```
function
[furnance_cost]=calc_cost_furnan
ce(QeeQ)
QeeQ=100;
Q=QeeQ*9.47*10^-10; % energy req
for gasification process QeeQ is
in J/hr and converted to Mbtu/hr
pm=0.49096; % density of EFB
(g/m3)
Fc=1; % based on assumption that
stainless steel materilas
MS=1491.70; %from Chemical
Engineering magazine
furnance_cost=(MS/280)*(5.52*10^
3)*(Q^0.85)*Fc;
end
```

Cost of Boiler

```
function
[boiler_cost]=calc_cost_boiler(s
teamflow1,steamflow2)
ST=(steamflow1+steamflow2);
MD=1000;
boiler_cost=(3.28*10^5)*(ST/MD)^
0.81;
```

```
end
```

Purchased Equipment Cost

```
function [PEC] =
calc_PEC2(PEC_pretreatment,PEC_gasifier,PEC_filter,PEC_scrubber,
PEC_psa,PEC_furnace,PEC_boiler)
PEC=PEC_pretreatment+PEC_gasifier+PEC_filter+PEC_scrubber+PEC_psa+PEC_furnace+PEC_boiler;
end
```

Fixed Capital Investment

```
function [FCI] = calc_FCI(PEC)
DC=3.778*PEC;
IC=0.4165*PEC;
FCI=DC+IC;
end
```

Total Production Cost

```
function [TPC] =
calc_TPC(FCI,efb,steamflow1,steamflow2)
rawcost=efb*0.015; % Assuming
efb in kg/hr and efb costs USD
0.015/kg
utility=12.90; % USD 12.90/kg.
Taken from P. Lv et al.
steamcost=(steamflow1+steamflow2)*0.002; % USD 0.002/kg. Taken
from Hamada Boiler Malaysia,
2008
catalystcost=efb*7.8279; % USD
7.8279/kg.  Taken from P. Lv et
al.
sorbentcost=efb*0.098; % USD
0.098/kg. Taken from iCheme
Website, 2002
OL=0.15*FCI;
supervision=0.15*OL;
repair=0.05*FCI;
TDPC=rawcost+utility+steamcost+catalystcost+sorbentcost+OL+supervision+repair;
TPC=TDPC;
end
```

Total Capital Investment

```
function [TCI] = calc_TCI(FCI)
WC=0.2*FCI;
TCI=FCI+WC;
end
```

Cost of Hydrogen Produced

```
function [hydrogencost] =
calc_hydrogencost(TCI,TPC,total_hydrogen)
TC=TCI+TPC;
hydrogencost=TC/total_hydrogen;
end
```

Optimization

```
% define the initial guess
independent variables for
optimization
X0=1;
% define the lower bounds for
independent variables
LB=[];
% define the upper bounds for
independent variables
UB=[];
% define the coefficients for
the linear inequality
constraints
A = [];
B = [];
% define the coefficients for
the linear equality constraints
Aeq = [];
Beq = [];
% define the options for the
optimization solver
options =
optimset('Algorithm','active-set','Display',
'iter','MaxFunEvals',1e6,'MaxIter',1e6, ...
    'TolFun',1e-6,'TolConSQP',1e-6,'TolX',1e-6,'FunValCheck','on');
% solving the optimization
problem
[X,FVAL,EXITFLAG,OUTPUT,LAMBDA,GRAD,HESSIAN]=fmincon(@calc_hydrogencost_drysocc,X0,A,B,Aeq,Beq,LB,UB,@calc_hydrogencost_drysocc_constraints,options);
```