M.SC. THESIS

Performance Evaluation of Gasifier based on Exergy Analysis

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DEDICATION

This thesis is dedicated to

My Grandfather

(for his support)

My Parents

(for their blessings)

and

My Friends

(who motivated me to complete this project)

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All praises to Allah Almighty who has provided me this opportunity and made it possible for me to complete this project.

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ABSTRACT

Gasification processes have received significant attention in recent years due to increasing world energy needs and growing environmental considerations. Gasification is a relatively environment friendly process but has low thermodynamic efficiency. Such thermodynamic inefficiencies and irreversibilities reduce the overall plant efficiency. Exergy analysis — a concept derived from the second law of thermodynamics — makes it possible to improve overall process efficiency by detecting and reducing thermodynamic irreversibilities in a process.

In this research project, an entrained-flow coal gasifier has been simulated using Aspen Plus® process simulator. First, a steady-state simulation model is developed and fine-tuned to match available experimental data. The results of this reference simulation are used as input for exergy analysis of the gasifier. The study then focuses on a systematic investigation of the influence of feedstock composition and operating conditions (including oxygen-to-coal and steam-to-coal ratios) on overall exergy efficiency of the gasifier. The outcome of this detailed analysis is a set of recommendations for choosing optimum gasification conditions for a given coal type.

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CHAPTER 1

INTRODUCTION

1.1. Problem Narrative

Rapid increase in urbanization and modernization have resulted in an ever-increasing demand for energy. The global energy consumption is projected to increase by 56% from 524 quadrillion British thermal units (Btu) in 2010 to 820 quadrillion Btu in 2040.[1] On the other hand, declining fossil fuel reserves have steadily pushed energy prices upwards. Increased energy demand and prices, coupled with growing environmental concerns, necessitate the development of more energy efficient and environment friendly processes to maintain the current pace and persistence of human achievements.

Coal is widely used for power generation because of its relative abundance and cost stability.[2] However, particulate emissions from direct combustion of coal pose serious environmental challenges. Gasification is an important thermochemical process for production of clean syngas — a mixture of hydrogen and carbon monoxide — from carbonaceous solid fuels, including coal, biomass, and municipal solid waste.[3] This is particularly important for effective utilization of low-quality feedstocks.[4] The syngas thus produced can be utilized in high-efficiency equipment, including gas turbines, internal combustion engines, and fuel cells.

The performance of thermal power plants has traditionally been evaluated through energetic performance criteria — electrical power output and thermal efficiency of coal-to-power conversion — based on the first law of thermodynamics. However, from the viewpoint of the second law of thermodynamics, irreversibilities in a process lead to increase in entropy and degradation in the quality of energy, ultimately resulting in low thermodynamic efficiency. To ensure a fair comparison between alternative processes and equipment designs, it is necessary to consider not only the quantity but also the quality of energy involved. Exergetic performance analysis, based on the second law of thermodynamics, is now increasingly used for the design, performance evaluation, and optimization of thermal power plants.[5]

The exergy, also called availability, is the maximum useful work obtained from a system at a given state in a given environment such that the system achieves chemical, mechanical, and thermal equilibrium with the environment.[6] Exergy analysis provides a measure of both the quantity and quality of energy involved in a process.[7] It can therefore be used to identify the performance bottlenecks and the sources of irreversibilities in a process. A reduction in exergy loss increases the energy availability and improves the overall process efficiency.

Through comprehensive exergy analysis of various sections of a coal-to-syngas system, Li et al.[8] have shown that considerable exergy destruction occurs in the coal gasification unit. Exergy analysis of an integrated gasification combined cycle (IGCC) plant by Lee et al.[9] exhibited similar results. Reducing the exergy destruction in the gasifier is therefore critical for improving the overall efficiency of syngas production from coal.

1.2. Scope and Objectives of this Project

Gasification is a thermochemical process in which a carbonaceous feedstock is converted into a gaseous product with useful heating value using controlled amount of a gasifying agent, typically air, oxygen, or steam.[3] This definition excludes complete combustion because the product flue gas has no residual heating value.[10-11] Because gasification involves partial, rather than complete, oxidation of the feedstock, the amount of oxygen must be carefully controlled to maintain an oxygen-deficient environment. The target is to convert carbon content of the feedstock into CO rather than CO_2, and hydrogen content of the feedstock into H_2 rather than H_2O. Both CO and H_2 are excellent gaseous fuels for use in gas turbines, internal combustion engines, and fuel cells. Similarly, in a gasification process, nitrogen content of the feedstock is converted into N_2 rather than NOx, and sulfur content of the feedstock is converted into H_2S and COS rather than SOx. The nitrogen and sulfur products produced during gasification are considerably easier to remove than those produced during complete combustion, making gasification an environment friendly alternative to direct combustion.

As explained above, reaction products change as the oxygen-to-carbon and oxygen-to-hydrogen ratios change from combustion to gasification conditions. This means that feedstock composition and moisture content play a critical role in determining the composition of the product syngas. Moreover, operating conditions including oxygen-to-coal and steam-to-coal ratios are important in controlling the extent of combustion reactions and the gasifier temperature, which ultimately affect the composition of the product syngas and its heating value. Kunze et al.[12] pointed out that irreversible entropy production during chemical conversion is the dominant cause of exergy destruction in a gasifier. Careful control of the gasifier operating conditions and the extent of gasification reactions is therefore critical for reducing exergy losses.

In this research project, an entrained-flow coal gasifier has been simulated using Aspen Plus® process simulator. First, a steady-state simulation model is developed and fine-tuned to match available experimental data. The results of this reference simulation are used as input for exergy analysis of the gasifier. The study then focuses on a systematic investigation of the influence of feedstock composition and operating conditions (including oxygen-to-coal and steam-to-coal ratios) on overall exergy efficiency of the gasifier. The outcome of this detailed analysis is a set of recommendations for choosing optimum gasification conditions for a given coal type.

1.3. Organization of this Thesis

Chapter 2, “Literature Review”, begins with a brief introduction to the gasification chemistry followed by a description of the salient features of various types of gasifiers. The chapter concludes with a discussion on reported simulation models and exergy analyses of entrained-flow coal gasifiers.

Chapter 3, “Development of a Simulation Model for an Entrained-Flow Coal Gasifier in Aspen Plus®”, outlines a step-by-step procedure for the development of reference simulation model.

Chapter 4, “Exergy Analysis”, begins with a detailed description of the procedure for calculation of the total exergy of a stream and the exergy efficiency of the overall system. The procedure is then applied to explore the effect of feedstock composition and operating conditions on overall exergy efficiency of the gasifier.

Chapter 5, “Conclusions and Future Research Directions” summarizes important findings of this project and identifies directions for further research on the topic.

CHAPTER 2

LITERATURE REVIEW

2.1. Gasification Chemistry

Gasification is a complex process involving a variety of physical and chemical processes. A typical gasification process involves:[13]

1. Preheating and drying
2. Thermal decomposition or pyrolysis
3. Partial combustion of some gases, vapors, and char
4. Gasification of decomposed products

It is important to emphasize that these steps overlap in a gasifier and there are no clear boundaries between the respective zones. However, for modeling purposes, it is often convenient to assume that these steps occur in a series in clearly defined zones.[14]

2.1.1. Preheating and Drying

Every kilogram of moisture in feedstock requires at least $2.25\ \mathrm{MJ}$ of energy from the gasifier to vaporize water. This energy loss quickly becomes a matter of concern for feedstocks with high moisture content. While little can be done about the inherent moisture content of the feedstock, external or surface moisture content should be removed from the feedstock before it is fed to the gasifier. For the production of syngas with reasonably high heating value, moisture content in gasifier feedstocks is generally limited to 10–20%.[15]

Upon entering the gasifier, the feed is preheated by heat from the hot zone below. The loosely bound moisture is irreversibly removed above $100\ ^\circ\mathrm{C}$. This is followed by evaporation of low-molecular-weight volatile compounds until the temperature reaches about $200\ ^\circ\mathrm{C}$.[13]

2.1.2. Pyrolysis

As the feed moves down the gasifier, its temperature continues to increase. The process of thermal degradation or pyrolysis occurs around $300-650\ ^\circ\mathrm{C}$ in the absence or very limited supply of oxidizing agent that does not permit gasification.[13] During pyrolysis, large complex molecules are broken into several smaller fragments. The product distribution depends on feedstock composition as well as operating conditions (including heating rate and temperature). Because biomass feedstocks are generally rich in volatiles, the role of pyrolysis is more important in biomass gasification than in coal gasification.[16] Pyrolysis products can be classified into three principle types:

1. Volatiles (hydrogen, carbon monoxide, carbon dioxide, water, and light hydrocarbons)
2. Liquids (heavy hydrocarbons and tar)
3. Solids (char/carbon and ash)

2.1.3. Partial Combustion of Volatiles

The gaseous products of pyrolysis are rapidly oxidized under the typical operating conditions of gasifiers. Typical reactions include:

$$\mathrm{CO}+0.5\mathrm{O_2}\rightarrow \mathrm{CO_2} \qquad \ldots(2.1)$$

$$\mathrm{H_2}+0.5\mathrm{O_2}\rightarrow \mathrm{H_2O} \qquad \ldots(2.2)$$

$$\mathrm{CH_4}+2\mathrm{O_2}\rightarrow \mathrm{CO_2}+2\mathrm{H_2O} \qquad \ldots(2.3)$$

$$\mathrm{C_6H_6}+7.5\mathrm{O_2}\rightarrow 6\mathrm{CO_2}+3\mathrm{H_2O} \qquad \ldots(2.4)$$

These oxidation reactions are highly exothermic and provide necessary heat for the endothermic gasification reactions.

2.1.4. Char Gasification

Gasification of char involves several reactions between the char carbon and the gasifying medium. Typical reactions include:[10,17]

$C + 0.5O_2 \rightarrow CO$ Gasification with oxygen …(2.5)

$C + H_2O \rightarrow CO + H_2$ Gasification with steam …(2.6)

$C + 2H_2 \rightarrow CH_4$ Gasification with hydrogen …(2.7)

$C + CO_2 \rightarrow 2CO$ Gasification with carbon dioxide …(2.8)

$C + O_2 \rightarrow CO_2$ Combustion with oxygen …(2.9)

Other reactions that take place under gasification conditions include methanation, steam reforming, and water-gas shift reaction.

$CO + 3H_2 \rightarrow CH_4 + H_2O$ Methanation …(2.10)

$2CO + 2H_2 \rightarrow CH_4 + CO_2$ Methanation …(2.11)

$CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O$ Methanation …(2.12)

$CH_4 + H_2O \rightarrow CO + 3H_2$ Reforming with steam …(2.13)

$CH_4 + 0.5O_2 \rightarrow CO + 2H_2$ Reforming with oxygen …(2.14)

$CO + H_2O \rightarrow CO_2 + H_2$ Water–gas shift reaction …(2.15)

2.2. Types of Gasifiers

Numerous gasifier designs have been commercialized over the years.[16] However, based on the flow pattern inside the gasifier, the locations of coal, steam, and air/oxygen inlets, and the locations of syngas and ash outlets, essentially all gasifiers can be categorized as one of the three generic types:[18]

1. Moving-bed gasifiers (counter-current reactors)
2. Fluidized-bed gasifiers (back-mixed reactors)
3. Entrained-flow gasifiers (plug-flow reactors)

2.2.1. Moving-Bed Gasifiers

A moving-bed gasifier (Figure 2.1) is essentially a counter-current reactor in which a bed of coal gradually moves downwards under the action of gravity while reacting with gases moving upwards through the bed. The incoming coal is first heated and dried near the top of the gasifier. The coal is then gradually devolatilized and gasified on its way toward the bottom of the gasifier. Because of the counter-current arrangement, oxygen consumption is relatively low.[11] However, excess steam is required to maintain the temperature below the ash-slagging temperature in the combustion zone near the bottom.[18] The temperature and composition of the syngas leaving the gasifier strongly depend on the temperature, composition, and moisture content of the feedstock. A major drawback of the moving-bed gasifiers is their inability to handle the presence of fines, especially if coupled with strong caking properties.

2.2.2. Fluidized-Bed Gasifiers

A fluidized-bed gasifier (Figure 2.2) is very similar to a mixed-flow reactor. By mixing the incoming coal particles with those already undergoing gasification, both heat and mass transfer rates are enhanced. However, due to a uniform distribution of converted, partially-

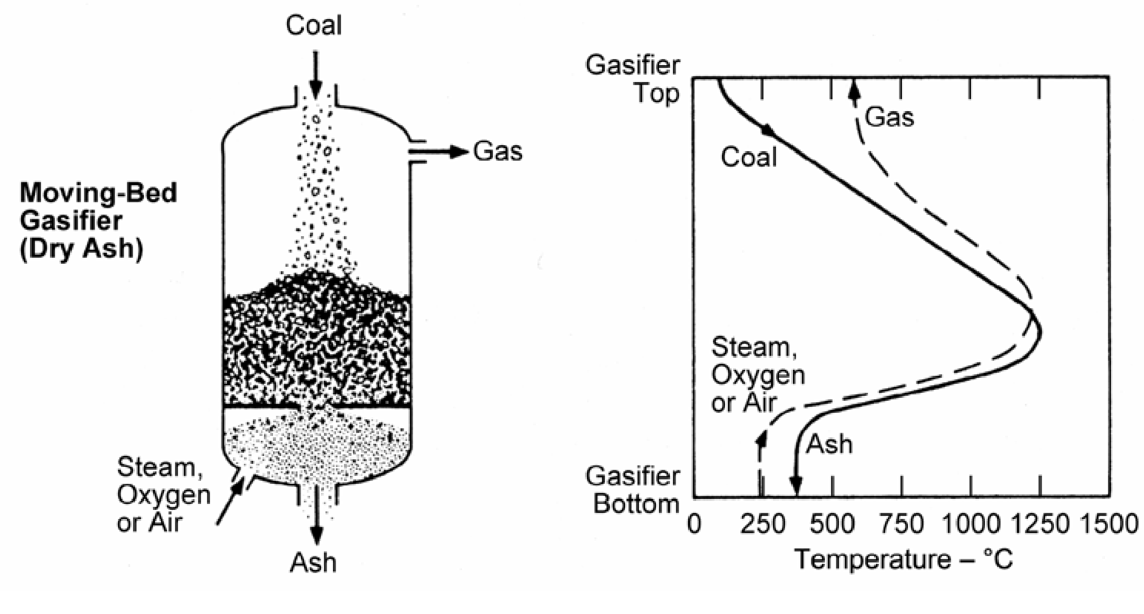

Figure 2.1. Schematic representation of a moving-bed gasifier and its temperature profile[18]

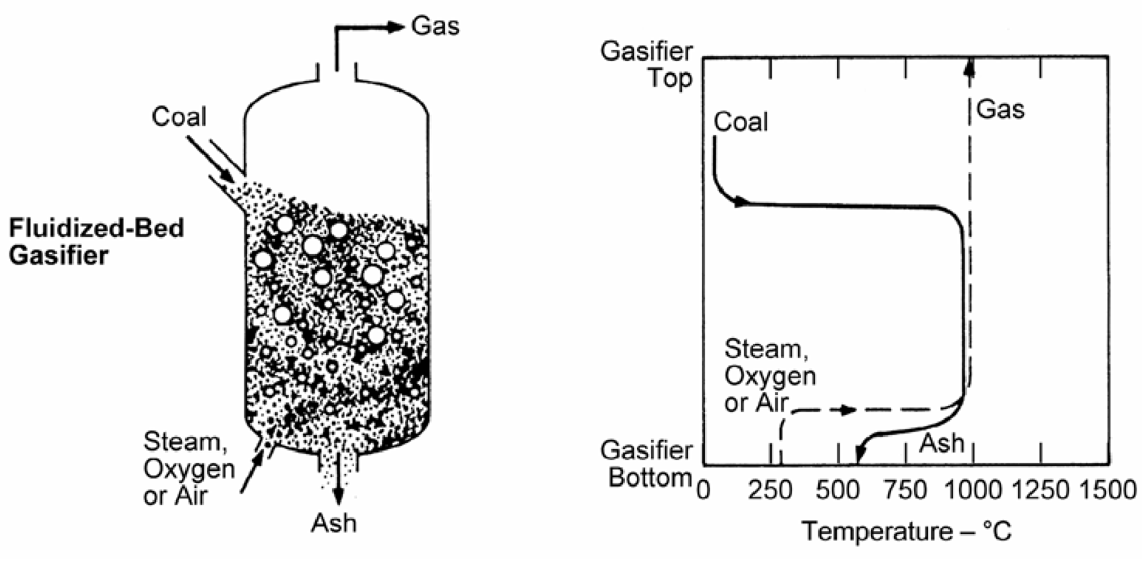

Figure 2.2. Schematic representation of a fluidized-bed gasifier and its temperature profile[18]

converted, and unconverted material in the reactor, some unconverted carbon leaves with the ash. To achieve desired level of conversion, it is often necessary to recycle the char. Similarly, very fine particles can become entrained with the product syngas and must be recycled using a cyclone. Because of the relatively moderate operating conditions and moderate requirements of oxygen and steam, fluidized-bed gasifiers are suitable for reactive feedstocks including low-rank coals and biomass.[11]

2.2.3. Entrained-Flow Gasifiers

In an entrained-flow gasifier (Figure 2.3), both the feedstock and the gasifying agent move co-currently through the reactor in a plug-flow arrangement. The particle size must be sufficiently small to allow entrainment in the gasifying medium. Given the short residence time (typically on the order of a few seconds), the reactor must be operated at sufficiently high temperature to ensure good conversion of carbon. As a result, entrained-flow gasifiers generally use oxygen as the oxidant and operate well-above the ash-slagging temperature.[18] Because of the very high operating temperature, the product syngas is nearly free of tar. However, it is necessary to cool the product syngas before cleaning.

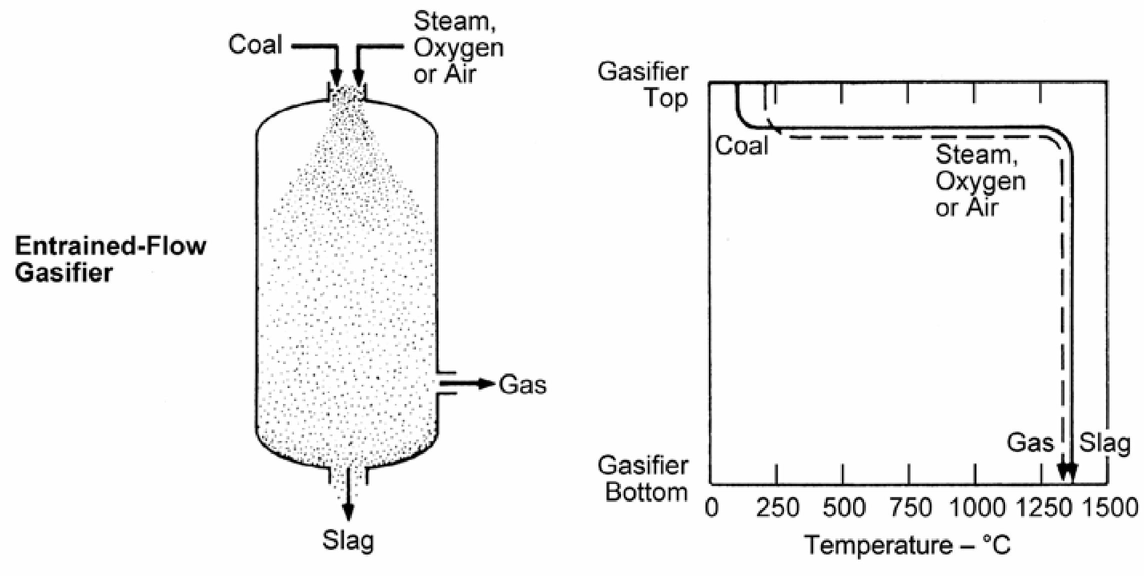

Figure 2.3. Schematic representation of an entrained-flow gasifier and its temperature profile[18]

Because of their large capacity, high carbon conversion, and ability to handle wide range of feedstocks, entrained-flow gasifiers are the most widely used gasifiers. In particular, Shell-and-Texaco entrained-flow gasifiers are used in nearly 75% of coal-fired power plants.[19]

2.3. Simulation Models of Entrained-Flow Coal Gasifiers

Wen and Chaung[20] were the first to develop a conceptual model for an entrained-flow gasifier. They divided the reactor into three zones: pyrolysis and volatile combustion zone, gasification and combustion zone, and gasification zone. Detailed material and energy balance equations for the system were then developed based on gasification kinetics and reactor hydrodynamics. The predicted temperature and composition profiles were validated against experimental data from the Texaco downflow pilot-scale gasifier. Sensitivity analysis with respect to the model parameters was used to find optimum operating conditions. Oxygen-to-fuel and steam-to-fuel ratios were identified as the most important process variables. Govind and Shah[21] further improved the model by including full momentum balance equations for the solid phase and confirmed the findings of Wen and Chaung.[20]

Ni and Williams[22] developed a multivariable model based on mass and energy balances and chemical equilibrium for the Shell entrained-flow coal gasifier. They identified oxygen-to-coal ratio and gasifier exit temperature as the most important process variables. Vamvuka et al.[23-24] developed a one-dimensional steady-state model for an entrained-flow coal gasifier based on thermogravimetric analysis data. They found that a high gasifier pressure and low steam-to-coal and oxygen-to-coal ratios are preferable operating conditions. Chen et al.[25-26] developed a comprehensive three-dimensional model for a $200\ \mathrm{ton/day}$ air-blown entrained-flow coal gasifier. The model predicted that the reactions in the gasifier can be roughly divided into devolatilization, gasification, and combustion zones. Furthermore, coal devolatilization and char oxidation were found to be the dominant carbon conversion reactions. Tremel and Spliethoff[27-29] developed a detailed model for gasification kinetics in entrained-flow coal gasification. They concluded that the overall rate of carbon conversion is strongly correlated with the rate of char conversion reactions. Watanabe et al.[30] investigated the effect of CO_2 injection on gasification characteristics and showed that the gas-phase oxidation reactions are the major source of heat for the endothermic gasification reactions. Moreover, gasification with steam (Equation (2.6)) was found to be the predominant heterogeneous reaction in the whole gasifier.

Process simulation software allow low-cost yet reliable solution of complex engineering problems by expressing the behavior of the process using fundamental laws of conservation of mass, energy, and phase equilibria. Aspen Plus® has been leading the development of process simulation models for a diverse range of unit operations. With the recent advances in Aspen Plus®, many efforts have been made to develop models for entrained-flow coal gasifiers.[31] Based on the underlying assumptions,[14] these models are either equilibrium-based or kinetics-based.

In the equilibrium-based models, all reaction zones are modeled using RGIBBS reactor based on minimization of the Gibbs free energy. Kunze and Spliethoff[32] developed a generic equilibrium-based entrained-flow gasifier model using Aspen Plus® and used it to compare alternative gasifier designs. Lee et al.[31] used the same approach to compare alternative burner designs for a bench-scale entrained-flow gasifier. Kong et al.[33] developed a three-stage equilibrium model for Texaco-type entrained-flow coal gasifiers. Jang et al.[34] developed a more detailed simulation model for GE entrained-flow coal gasifier. The model was validated using data from the Integrated Gasification Combined Cycle Project at the Tampa Electric Polk Power Station.[35] It was then used to study the gasification characteristics of Indonesian bituminous coal (KIDECO) and its blend with biomass. Oxygen-to-coal ratio was found to be the most important process parameter, whereas gasifier temperature and pressure showed little effect on the yield of syngas.

Kinetics-based models are superior to equilibrium-based models because they do not require the assumption of long residence time. However, they are considerably more complicated to develop because each reaction zone must be modeled using full set of mass and energy balance equations. Examples of such models include the works of Biagini et al.[36] and Adeyemi and Janajreh.[37]

Biagini et al.[36] developed a kinetics-based multizone model using separate blocks for preheating, devolatilization, combustion, gasification, and quenching zones. The model was compared with the standard RGIBBS equilibrium-based model and showed clear improvements in terms of quantification of tar, residual char, and heat recovery. Adeyemi and Janajreh[37] developed a similar kinetics-based non-empirical model for entrained-flow gasification of Kentucky coal and wood waste. The model included drying, pyrolysis, volatile combustion, and gasification zones and showed good agreement with the experimental data.

2.4. Exergy Analyses of Entrained-Flow Coal Gasifiers

Exergy analysis provides a measure of both the quantity and quality of energy involved in a process.[7] It can therefore be used to identify those components of a system where considerable exergy destruction occurs. Since chemical reactions, heat transfer, mixing, and friction are the predominant sources of irreversibilities in process equipment, a detailed exergy analysis can also identify the underlying cause of exergy destruction in a process. For gasification processes, overall exergy efficiency is a function of the type of gasifier, composition of the feedstock, gasifying agent, and operating temperature and pressure of the gasifier.

Prins et al.[38] used exergy analysis to show that gasification has higher thermodynamic efficiency than slow pyrolysis and combustion. They also explored the effect of using air and steam as gasifying agents and concluded that gasification with steam is more suitable for production of methane-rich syngas, whereas gasification with oxygen is more suitable if carbon monoxide and hydrogen are the desired products. Prins et al.[39] explored the effect of feedstock composition on exergy efficiency of gasifiers and recommended optimum operating temperatures for various feedstocks. Ptasinski et al.[40] showed that the gasification of coal has higher exergy efficiency than the gasification of solid biomass. Karamarkovic and Karamarkovic[41] showed that high moisture content in gasifier feed resulted in low exergy efficiency of biomass gasification and recommended to maintain the moisture content around 10%. They also showed that overall exergy efficiency of the gasifier decreased at higher operating temperatures but increased at higher operating pressures.

Kunze et al.[12] performed structured exergy analysis of an IGCC plant and showed that almost 80% of the total exergy destruction in the whole plant occurred in just 4 units: gas turbine, gasifier, acid-gas removal unit, and CO shift reactor. Similar results were obtained by Liszka et al.[42] from exergy analysis of a coal-to-hydrogen plant. Lee et al.[9] performed detailed exergy analysis of an IGCC plant with an entrained-flow coal gasifier and showed that most exergy destruction occurred in units where chemical reactions took place, i.e., gasifier and gas turbine. Through comprehensive exergy analysis of various sections of a coal-to-syngas system, Li et al.[8] showed that the gasification unit was the largest contributor to total exergy destruction in the whole process.

CHAPTER 3

DEVELOPMENT OF A SIMULATION MODEL FOR AN ENTRAINED-FLOW COAL GASIFIER IN ASPEN PLUS®

3.1. Assumptions

The main objective of this work is to systematically investigate the effect of feedstock composition and operating conditions on the overall exergy efficiency of an entrained-flow coal gasifier. In the first step, a steady-state simulation model is developed using Aspen Plus® process simulator (Version 8.6). Since a complete gasifier model is not directly available in Aspen Plus®, different unit operations are combined to represent the overall process. The gasifier is divided in four zones (Figure 3.1):

1. Drying zone
2. Pyrolysis zone
3. Volatile combustion zone
4. Char gasification zone

An equilibrium-based approach is used for modeling reactions occurring in each zone. Additional assumptions include:

1. The process is at steady state.
2. Pressure drop in all zones is negligible.
3. Char consists of carbon and ash.
4. Tar is modeled using benzene as model compound.

3.2. Development of the Entrained-Flow Coal Gasifier Model

The specific steps for development of the simulation model in Aspen Plus® are as follows:

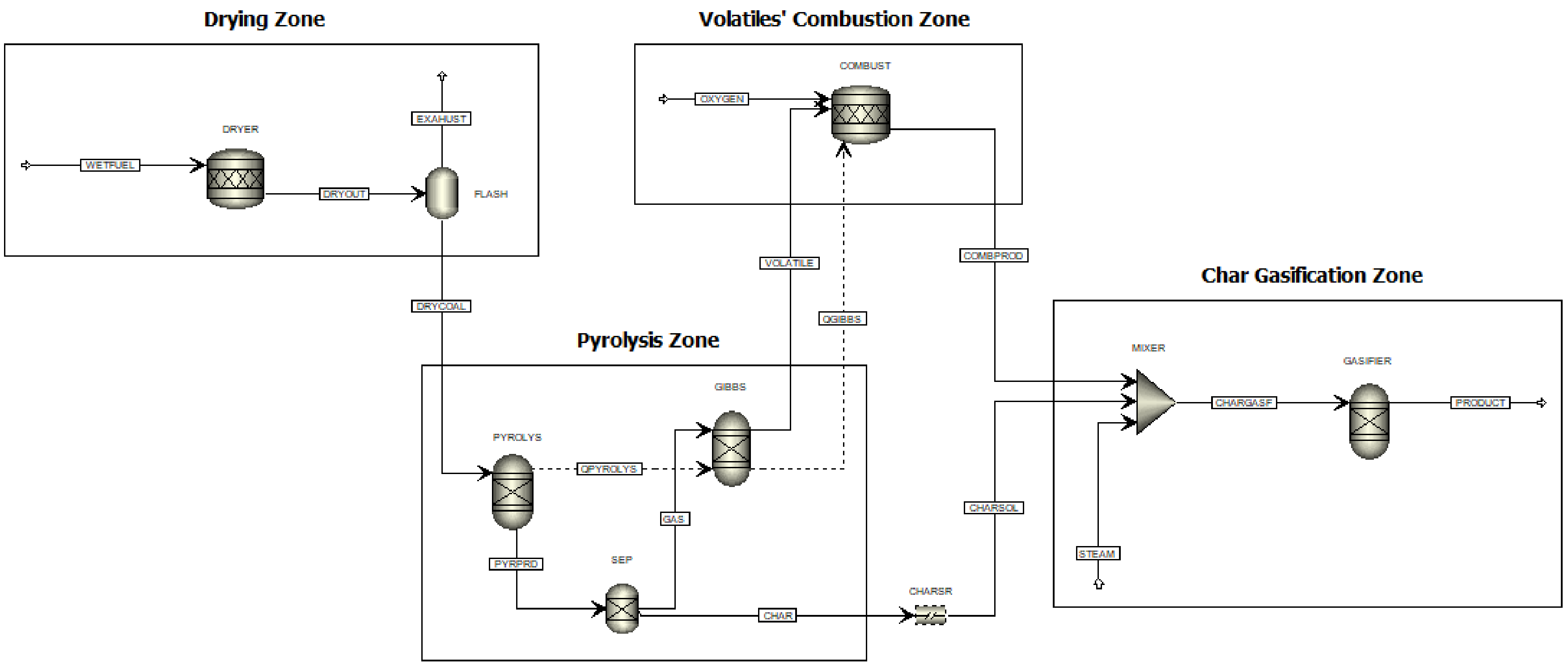

Figure 3.1. Schematic representation of the entrained-flow coal gasifier in Aspen Plus®

Table 3.1. Components' specification

Component ID	Type	Name	Alias
H2O	Conventional	Water	H2O
N2	Conventional	Nitrogen	N2
O2	Conventional	Oxygen	O2
H2	Conventional	Hydrogen	H2
CO	Conventional	Carbon monoxide	CO
CO2	Conventional	Carbon dioxide	CO2
CH4	Conventional	Methane	CH4
H2S	Conventional	Hydrogen sulfide	H2S
C6H6	Conventional	Benzene	C6H6
C	Solid	Carbon graphite	C
S-S	Solid	Sulfur	S
COAL	Nonconventional	---	---
ASH	Nonconventional	---	---

1. All components are added to the simulation (Table 3.1).
2. SRK (Soave–Redlich–Kwong) property package is used for all conventional components. HCOALGEN and DCOALIGT are used for non-conventional components.
3. MIXCINC is selected as global stream class. The coal feed is fully specified using proximate, ultimate, and sulfur analyses.
4. The drying zone is represented using an RSTOIC reactor block and a FLASH2 separator block.
5. The gasification zone is represented using RYIELD and RGIBBS reactor blocks. In the first step, an RYIELD reactor block breaks down non-conventional components into conventional elements. In the second step, an RGIBBS reactor block determines the equilibrium composition of volatiles based on minimization of the total Gibbs free energy of the system. The char produced in this zone is directly sent to the char

gasification zone, whereas the gaseous products are sent to the volatile combustion zone.

6. The volatile combustion zone is modeled using an RSTOIC reactor block for oxidation reactions with oxygen.
7. The char gasification zone is modeled using an RGIBBS reactor block with steam as the gasifying agent.

CHAPTER 4

EXERGY ANALYSIS

4.1. Methodology for Exergy Analysis

The total exergy of a material stream, $E\left[\mathrm{kW}\right]$, is a product of its molar exergy, $e\left[\mathrm{kJ/mol}\right]$, and molar flow rate, $\dot{m}\left[\mathrm{mol/s}\right]$.

$$E\left[\mathrm{kW}\right]=\dot{m}\left[\mathrm{mol/s}\right]\cdot e\left[\mathrm{kJ/mol}\right] \qquad \ldots(4.1)$$

When kinetic and potential exergy terms are neglected, the molar exergy of a material stream includes only physical and chemical exergies.

$$e=e^{ph}+e^{ch} \qquad \ldots(4.2)$$

The molar physical exergy, $e^{ph}\left[\mathrm{kJ/mol}\right]$, of a material stream is calculated using its molar enthalpy and molar entropy relative to a reference environment.

$$e^{ph}=\left(h-h_0\right)-T_0\left(s-s_0\right) \qquad \ldots(4.3)$$

where $T_0\left[\mathrm{K}\right]$ is the reference temperature, and $P_0\left[\mathrm{Pa}\right]$ is the reference pressure. $h\left[\mathrm{kJ/mol}\right]$ and $h_0\left[\mathrm{kJ/mol}\right]$ are molar enthalpies of the stream at actual conditions $\left(T,P\right)$ and reference conditions $\left(T_0,P_0\right)$, respectively. Similarly, $s\left[\mathrm{kJ/\left(mol\cdot K\right)}\right]$ and $s_0\left[\mathrm{kJ/\left(mol\cdot K\right)}\right]$ are molar entropies of the stream at actual and reference conditions, respectively. In this work, $T_0=298.15\ \mathrm{K}$ and $P_0=101,325\ \mathrm{Pa}$ have been selected as reference conditions.

The values of molar enthalpy and molar entropy at actual conditions are obtained from the converged steady-state simulation model. The corresponding values at reference conditions are determined by changing the temperature and pressure of the stream to reference conditions using a duplicator block coupled with a simple heater/cooler model.

Table 4.1. Standard chemical exergies of gas-phase components at $298.15\ \mathrm{K}$ and $101{,}325\ \mathrm{Pa}$ [43]

Component	$e^{ch}\ (\mathrm{kJ/mol})$	**Component**	$e^{ch}\ (\mathrm{kJ/mol})$
H_2O	9.50	N_2	0.72
O_2	3.97	H_2	236.10
CO	275.10	CO_2	19.87
CH_4	831.65	H_2S	812.00
C_6H_6	3,303.60	C graphite	410.26
S rhombic	609.60		

The molar chemical exergy, $e^{ch}\ [\mathrm{kJ/mol}]$, of a material stream is a function of its composition.

$$e^{ch} = \sum x_i e_i^{ch} + RT_0 \sum x_i \cdot \ln x_i \qquad \ldots(4.4)$$

where x_i is the mole fraction of component i in the stream, $e_i^{ch}\ [\mathrm{kJ/mol}]$ is the standard molar chemical exergy of component i, and R is the gas constant in appropriate units. The values of standard molar chemical exergies of all components in the system are listed in Table 4.1.

Specific exergy of coal can be calculated using the empirical correlation developed by Ghamarian and Cambel.[44]

$$e_{coal}\ [\mathrm{MJ/kg}] = \begin{cases} +443.35208n_C + 105.30292n_H \\ -184.17053n_O + 32.65797n_N \\ +513.159n_S \end{cases} \quad \text{for} \quad \frac{n_O}{n_C} \le 0.50 \qquad \ldots(4.5)$$

where n represents the number of moles of an element per kg of coal.

Finally, overall exergy efficiency of the gasifier is calculated as

$$\eta_E\ [\%] = \frac{E_{out}}{E_{in}} \times 100 = \frac{E_{syngas}}{E_{coal} + E_{oxygen} + E_{steam}} \times 100 \qquad \ldots(4.6)$$

Heating value of the product syngas is calculated using the expression from Karamarkovic and Karamarkovic.[41]

$$\mathrm{LHV_{syngas}}\left[\mathrm{kJ/kmol}\right] = 282,993\mathrm{x_{CO}} + 802,303\mathrm{x_{CH_4}} + 241,827\mathrm{x_{H_2}} \qquad \ldots(4.7)$$

4.2. Model Validation

The Aspen Plus® gasifier model (Chapter 3) was validated using data from the Texaco downflow pilot-scale gasifier.[20] The properties of the coal feed (coal 1) and operating conditions are listed in Table 4.2 and Table 4.3, respectively. Table 4.4 presents a comparison of the predicted and measured product syngas composition.

Table 4.2. Feedstock characterization

	Coal 1[20]	**Coal 2**	**Coal 3**
Proximate analysis, wt. %			
Moisture	0.20	4.58	42.55
Fixed carbon	58.01	39.16	38.61
Volatile matter	26.46	52.72	13.40
Ash	15.53	8.12	5.44
Ultimate analysis, wt. %			
Carbon	74.05	77.76	60.24
Hydrogen	6.25	5.24	6.68
Nitrogen	0.71	1.47	0.34
Sulfur	1.77	2.62	1.55
Oxygen	1.32	4.79	25.75
Heating value, MJ/kg	31.98	31.95	24.26

Table 4.3. Operating conditions for model validation[20]

Coal feed rate, g/s	76.66
Oxygen-to-coal ratio, g/g	0.866
Steam-to-coal ratio, g/g	0.241
Gasifier pressure, atm	24.0

Table 4.4. A comparison of the predicated and measured product syngas composition

(mole fraction)	**Measured[20]**	**Predicted**
CO	0.5757	0.5758
H_2	0.3913	0.3821
CO_2	0.0295	0.0295
CH_4	0.0012	0.0045
H_2S	0.0006	0.0055
N_2	0.0012	0.0025

4.3. Evaluation and Optimization of Exergy Efficiency

After model validation, steady-state simulation results are used to calculate overall exergy efficiency of the gasifier using the procedure described in Section 4.1. Many feedstock characteristics and operating conditions influence the overall performance of the gasifier. For example:

1. High moisture content in feed requires considerable amount of energy to completely evaporate.
2. An excess of oxygen moves the process from gasification to combustion regime and reduces the heating value of the product syngas.
3. An excess of steam absorbs considerable amount of sensible heat from the reaction system and lowers the reaction temperature.

The optimum operating conditions strongly depend on the feedstock composition. In this work, these effects are studied using three different coals (Table 4.2). Coal 1 has high fixed-carbon content, high heating value, and low moisture content. Coal 2 has comparable heating value but has somewhat higher moisture content and is rich in volatile matter. Coal 3 has high moisture content and low heating value.

4.3.1. Effect of Oxygen-to-Coal Ratio

Oxygen is used in gasifier for combustion of volatile products of pyrolysis. These oxidation reactions are highly exothermic and provide necessary heat for the endothermic gasification reactions. In general, increasing the oxygen-to-coal ratio results in an increase in the CO content of the product syngas as well as an increase in the overall exergy efficiency of the gasifier. However, a high oxygen-to-coal ratio can shift the process from gasification to combustion regime resulting in low-quality product syngas as well as lower exergy efficiency of the gasifier.

Figures 4.1–4.3 summarize the effect of oxygen-to-coal ratio on product syngas composition and overall exergy efficiency of the gasifier. High oxygen-to-coal ratio is desirable for coal 1 with a maximum exergy efficiency of 84% for oxygen-to-coal ratio of 0.87. The product syngas contains ~59% CO and ~36% H_2 content. Similarly, high oxygen-to-coal ratio is desirable for coal 2 with a maximum exergy efficiency of 80.7% for oxygen-to-coal ratio of 0.87. The product syngas contains ~66% CO and ~31% H_2 content. On the other hand, because of the high moisture content, low oxygen-to-coal ratio is desirable for coal 3 with a maximum exergy efficiency of 59.8% for oxygen-to-coal ratio of 0.3. The product syngas contains large H_2O and CO_2 content, especially at high oxygen-to-coal ratios.

4.3.2. Effect of Steam-to-Coal Ratio

Steam is used in gasifier for char gasification. In general, increasing the steam-to-coal ratio results in an increase in the overall exergy efficiency of the gasifier. However, an excess of steam can lower the gasifier temperature and result in a decrease in the exergy efficiency.

Figures 4.4–4.6 summarize the effect of steam-to-coal ratio on product syngas composition and overall exergy efficiency of the gasifier. For both coal 1 and coal 2, increasing the steam-to-coal ratio increases the overall exergy efficiency of the gasifier. The maximum exergy efficiency observed for coal 1 is 84% for a steam-to-coal ratio of 0.16. The maximum exergy efficiency observed for coal 2 is 80.7% for a steam-to-coal ratio of 0.05. Further increase in steam-to-coal ratio results in a slight decrease in the overall exergy efficiency. Because of the high moisture content, considerably low efficiency is observed for coal 3, which remains constant at approximately 57.5%. In all cases, an increase in the steam-to-coal ratio results in an increase in H_2O and CO_2 content and a decrease in H_2 and CO content of the product syngas.

Table 4.5 summarizes the optimum operating conditions to achieve maximum exergy efficiency for gasification of different coals studied in this project. Coal 3 produces syngas with very low heating value. This is not surprising considering the high H_2O and CO_2 content in the product syngas. We conclude that it is necessary to pre-dry coal 3 before feeding to the gasifier.

Table 4.5. Optimum operating conditions for gasification of different coals

	Coal 1	**Coal 2**	**Coal 3**
Exergy of feedstock, MJ/kg	34.04	34.04	25.91
Oxygen-to-coal ratio, g/g	0.87	0.87	0.3
Steam-to-coal ratio, g/g	0.16	0.05	0.01
Product syngas heating value, MJ/m^3	52.31	45.38	3.75
Total exergy in, MW	264.88	263.87	200.24
Total exergy out, MW	222.54	212.87	119.82
Exergy loss, MW	42.34	51.00	80.42
Overall exergy efficiency, %	84.0	80.7	59.8

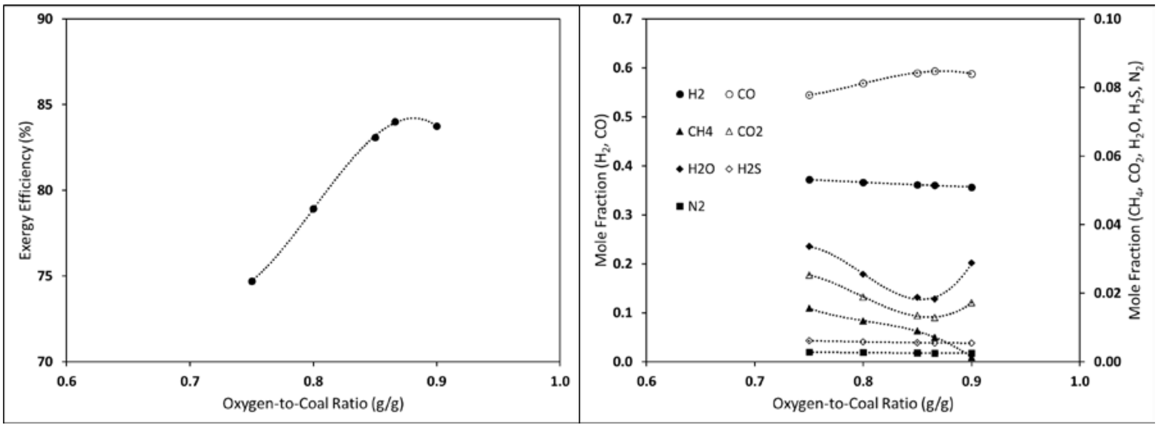

Figure 4.1. Effect of oxygen-to-coal ratio on overall exergy efficiency of the gasifier and product syngas composition for coal 1

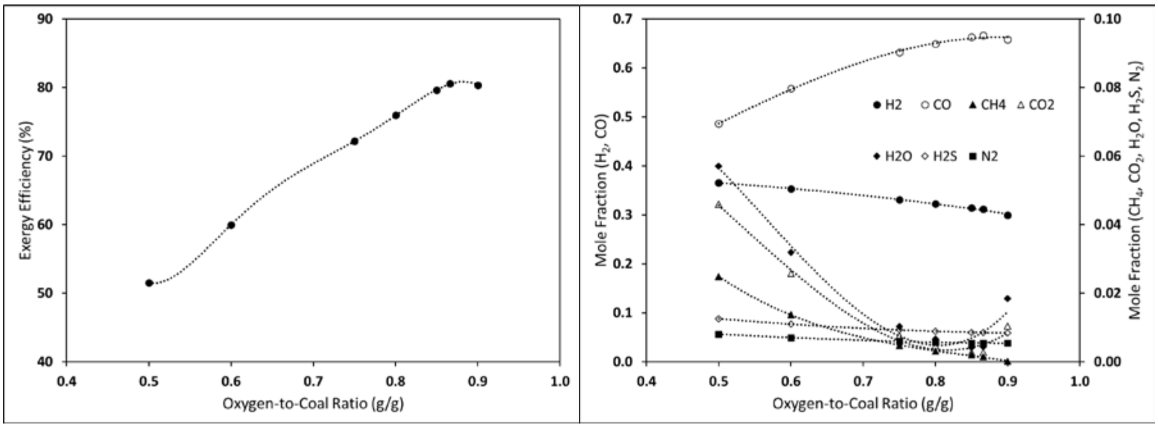

Figure 4.2. Effect of oxygen-to-coal ratio on overall exergy efficiency of the gasifier and product syngas composition for coal 2

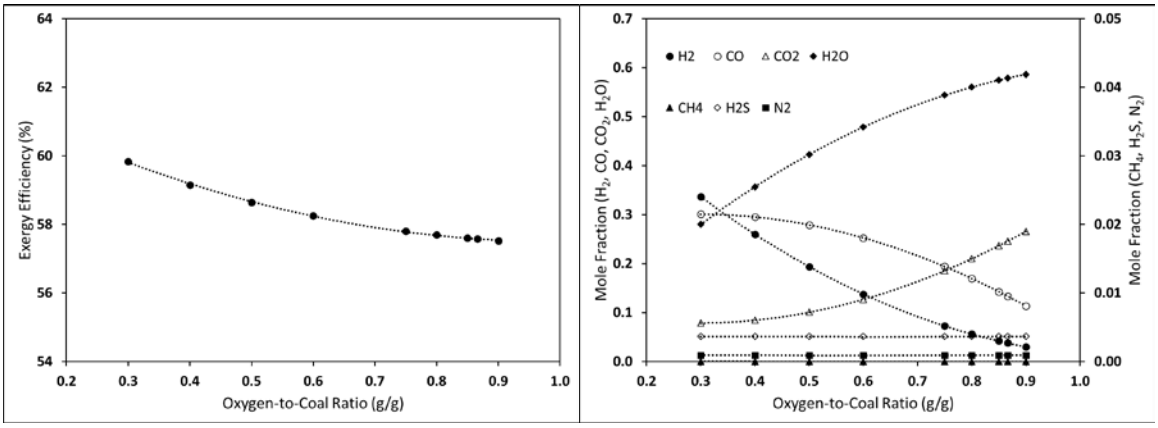

Figure 4.3. Effect of oxygen-to-coal ratio on overall exergy efficiency of the gasifier and product syngas composition for coal 3

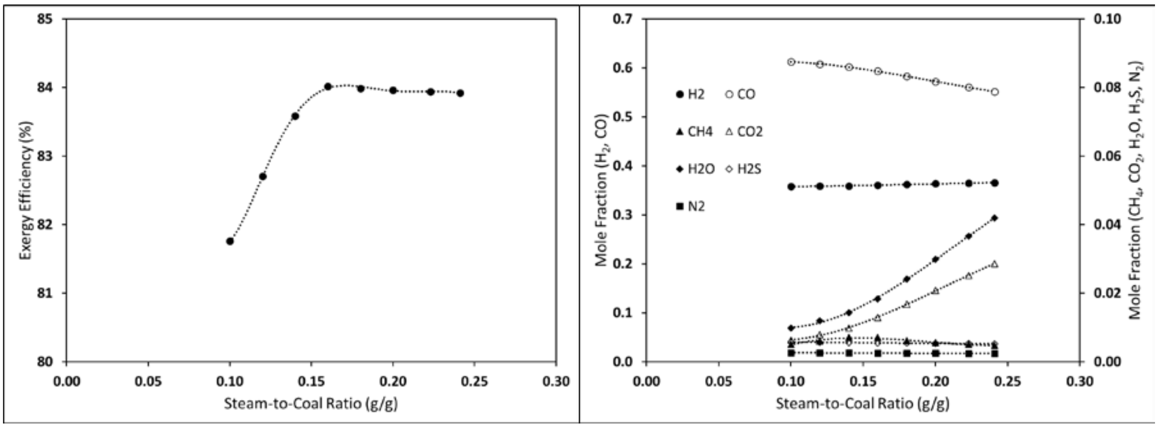

Figure 4.4. Effect of steam-to-coal ratio on overall exergy efficiency of the gasifier and product syngas composition for coal 1

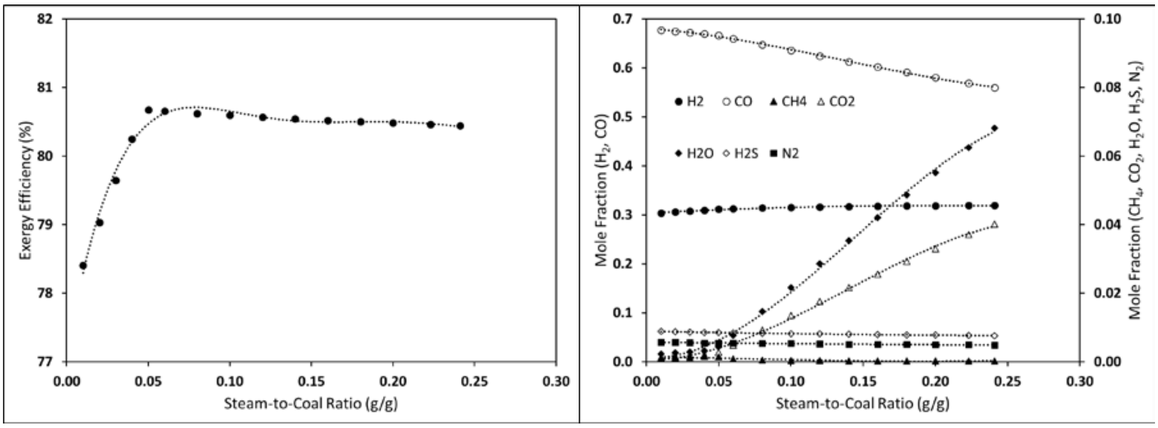

Figure 4.5. Effect of steam-to-coal ratio on overall exergy efficiency of the gasifier and product syngas composition for coal 2

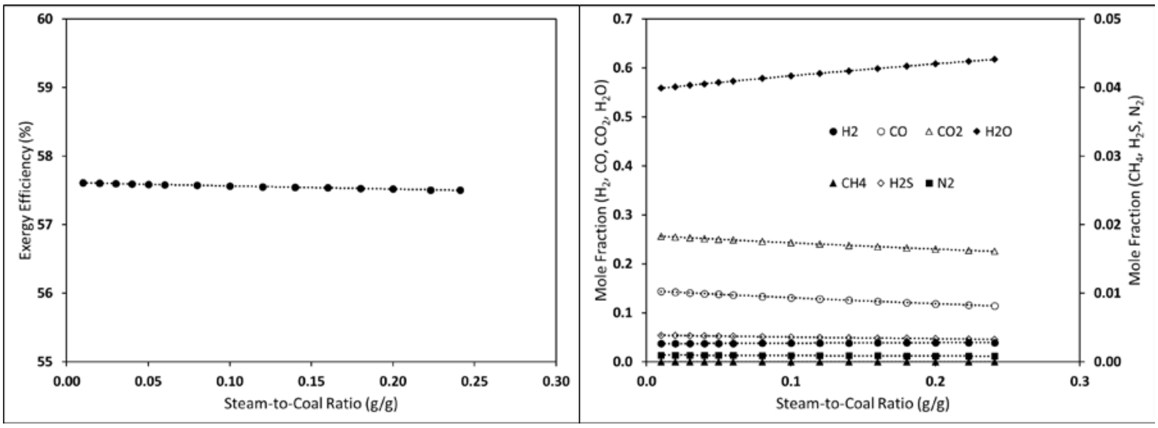

Figure 4.6. Effect of steam-to-coal ratio on overall exergy efficiency of the gasifier and product syngas composition for coal 3

CHAPTER 5

CONCLUSIONS AND FUTURE RESEARCH DIRECTIONS

5.1. Conclusions

Exergy analysis is an effective technique for thermodynamic performance evaluation. By taking both the quantity and quality of energy into consideration, exergy analysis allows identification of the type, magnitude, and cause of irreversibilities in a system.

In this project, a steady-state simulation model of an entrained-flow coal gasifier was developed using Aspen Plus® process simulator. The gasifier was divided in drying, pyrolysis, volatile combustion, and gasification zones and an equilibrium-based approach was adopted for modeling reactions occurring in each zone. The model was validated using data from the Texaco downflow pilot-scale gasifier and then used to optimize oxygen-to-coal and steam-to-coal ratios for three different coals.

Coal 1 with high fixed-carbon content, high heating value, and low moisture content was found to be the most suitable feedstock. The maximum exergy efficiency of the gasifier operating with coal 1 feed was found to be 84%. The product syngas was rich in H_2 and CO and had a heating value of $52.31\,\mathrm{MJ/m^3}$. Coal 2 with moderate moisture content and high volatile matter content was found to be a reasonably good feedstock. The maximum exergy efficiency of the gasifier operating with coal 2 feed was found to be 80.7%. The product syngas was rich in H_2 and CO and had a heating value of $45.38\,\mathrm{MJ/m^3}$. Coal 3 with high moisture content was found to be a poor feedstock. The maximum exergy efficiency of the gasifier operating with coal 3 feed was found to be only 59.8%.The product syngas was rich in H_2O

and CO_2 and had a heating value of only $3.75\ \mathrm{MJ/m^3}$. This implies that it is necessary to pre-dry coal 3 before feeding to the gasifier.

For gasifiers operating with coal 1 and coal 2 feeds, an increase in the oxygen-to-coal and steam-to-coal ratios resulted in an increase in the overall exergy efficiency up to a limit. Further increase in oxygen-to-coal and steam-to-coal ratios resulted in a slight decrease in the overall exergy efficiency of the gasifier. On the other hand, for the gasifier operating with coal 3 feed, the overall exergy efficiency was found to be almost independent of oxygen-to-coal and steam-to-coal ratios.

5.2. Future Research Directions

Comparison of different coals for use in an entrained-flow gasifier and optimization of oxygen-to-coal and steam-to-coal ratios has been the primary focus of this project. Other areas of interest identified during this project include:

1. Kinetics-based gasifier model may be developed to properly account for residence time and remove the assumption of equilibrium reactor.
2. Different types of gasifiers may be compared based on their exergy efficiency for a given feedstock.

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