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ENERGY OPTIMIZATION OF STEAM GASIFICATION IN A FLUIDIZED BED REACTOR BY
ASPEN PLUS

Mr. Siripong Limprachaya



A Thesis Submitted in Partial Fulfillment of the Requirements
for the Degree of Master of Engineering Program in Chemical Engineering
Department of Chemical Engineering
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ศิริพงศ์ ลิ้มปรีชญา : การออปติไมซ์พลังงานของแก๊สซิฟิเคชันด้วยไอน้ำในเตาปฏิกรณ์ชนิดฟลูอิดไคซ์เบดด้วยแอสเพนพลัส (ENERGY OPTIMIZATION OF STEAM GASIFICATION IN A FLUIDIZED BED REACTOR BY ASPEN PLUS) อ.ที่ปรึกษาวิทยานิพนธ์หลัก: ศ. ดร.ไพศาล กิตติศุภกร, หน้า.

แก๊สซิฟิเคชันถูกพิจารณาให้เป็นกระบวนการที่เหมาะสมในการผลิตแก๊สเชื้อเพลิงด้วยสิ่งปฏิกูลจากคริวรีนหรือไบโอแมส ซึ่งกระบวนการที่เกิดขึ้นในแก๊สซิฟายเออร์ประกอบไปด้วยโซนไพโรไลซิส โซนการเผาไหม้ของซาร์ และโซนแก๊สซิฟิเคชันของซาร์ จุดประสงค์ของการศึกษานี้เพื่อทำให้ออปติไมซ์พลังงานของแก๊สซิฟิเคชันด้วยไอน้ำในเตาปฏิกรณ์ชนิดฟลูอิดไคซ์เบด โดยการหาสถานะที่ทำให้ปฏิกิริยาเคมีเกิดขึ้นได้โดยปราศจากการให้พลังงานภายนอก ซึ่งทำได้โดยการปรับเปลี่ยนอุณหภูมิของแก๊สซิฟิเคชัน อัตราส่วนของอากาศต่อไบโอแมส และอัตราส่วนของไอน้ำต่อไบโอแมสภายใต้เงื่อนไขเปอร์เซ็นต์การเกิดปฏิกิริยาของซาร์และเปอร์เซ็นต์แก๊สคาร์บอนไดออกไซด์ยังคงอยู่ในเกณฑ์โดยที่มากกว่า 70 เปอร์เซ็นต์ และน้อยกว่า 20 เปอร์เซ็นต์โดยปริมาตร ตามลำดับ แบบจำลองกระบวนการแก๊สซิฟิเคชันด้วยไอน้ำถูกเขียนขึ้นและตรวจสอบความถูกต้องด้วยการเปรียบเทียบผลลัพธ์กับข้อมูลจากการทดลอง หลังจากนั้นการทดลองด้วยแบบจำลองกระบวนการสำเร็จรูปได้ถูกจัดเตรียมไว้ถึง 48 รอบ โดยในแต่ละรอบอัตราส่วนของอากาศต่อไบโอแมสและอัตราส่วนของไอน้ำต่อไบโอแมสจะถูกควบคุมให้คงที่แล้วจึงทำการหาค่าอุณหภูมิของแก๊สซิฟิเคชันที่ทำให้เกิดสถานะที่ทำให้ปฏิกิริยาเคมีเกิดขึ้นได้โดยปราศจากการให้พลังงานภายนอก อัตราส่วนของอากาศต่อไบโอแมสถูกควบคุมในช่วง 0 – 0.31 อัตราส่วนของไอน้ำต่อไบโอแมสถูกควบคุมในช่วง 0 – 4.49 และอุณหภูมิของแก๊สซิฟิเคชัน 600 – 1,000 องศาเซลเซียส ในที่สุดค่าออปติไมซ์ของการศึกษานี้คืออุณหภูมิของแก๊สซิฟิเคชันที่ 911 องศาเซลเซียส อัตราส่วนของอากาศต่อไบโอแมสที่ 0.18 และอัตราส่วนของไอน้ำต่อไบโอแมสที่ 1.78 ซึ่งทำให้ได้เปอร์เซ็นต์การเกิดปฏิกิริยาของซาร์และเปอร์เซ็นต์แก๊สคาร์บอนไดออกไซด์อยู่ที่ 91.03 เปอร์เซ็นต์ และน้อยกว่า 15.18 เปอร์เซ็นต์โดยปริมาตรตามลำดับ

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The gasification process is considered as an effective combustible gas production from municipal solid waste or biomass. Chemical reactions of this process can be separated into three reaction zones as pyrolysis zone, volatile combustion zone, and char gasification zone. The aim of this study was to optimize the required energy used in a steam gasification process by considering three operating parameters (gasification temperature, equivalence ratio, and steam-to-biomass ratio) in order to achieve an energy self-sufficient condition under the criteria that the carbon conversion efficiency must be more than 70 percentages, and carbon dioxide oxide gas is lower than 20 volumatic percentages. The simulation model of steam gasification process was done and validated with the experimental data according to the research by Nikoo & Mahinpey (2008). The series of RYIELD reactor, RGIBBS reactor, and RCSTR reactor represented all chemical reactions which occurred in fluidized bed gasifier. Forty-eight batches of simulation test run were set in order to perform energy optimization with several sets of operating parameters. Equivalence ratio was varied from 0 to 0.31, and steam-to-biomass ratio was varied from 0 to 4.49. Then, gasification temperature was properly selected in range of 600 – 1000 °C to obtain the energy self-sufficient condition. Finally, the optimum point of simulation test run is at gasification temperature is 911 °C, equivalence ratio is 0.18, and steam-to-biomass ratio is 1.78. This operating point gives the maximum of carbon conversion efficiency at 91.03 percentages, and carbon dioxide oxide gas is still in criteria at 15.18 volumatic percentages.

Department: Chemical Engineering Student's Signature

Field of Study: Chemical Engineering Advisor's Signature

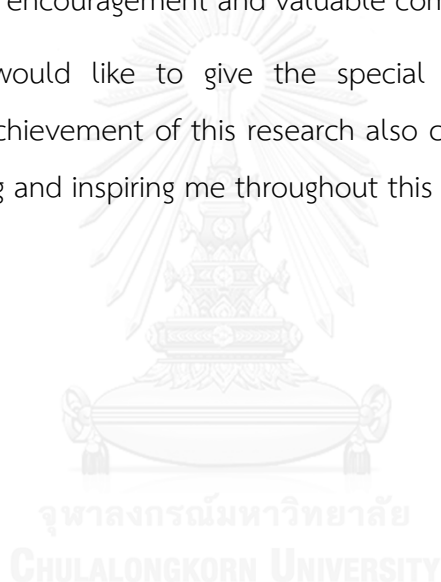
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LIST OF NOMENCLATURES

E_i	activation energy for rate constant of reaction i, $\frac{\text{kJ}}{\text{mol}}$
E_{CO}	activation energy for rate constant of char combustion reaction, $\frac{\text{kJ}}{\text{mol}}$
E_{SG}	activation energy for rate constant of char steam gasification reaction, $\frac{\text{kJ}}{\text{mol}}$
ΔG_i°	standard Gibb free energy change, $\frac{\text{kJ}}{\text{mol}}$
G_i	Gibb free energy of component i, $\frac{\text{kJ}}{\text{mol}}$
$\Delta H_{25^\circ\text{C}}$	standard enthalpy change of reaction (at 25°C), $\frac{\text{kJ}}{\text{mol}}$
K	equilibrium constant of the chemical reaction, dimensionless
k_i	rate constant for reaction i, $\text{s}^{-1} \text{atm}^{-1}$
k_{CO}	rate constant for char combustion reaction, $\text{s}^{-1} \text{atm}^{-1}$
k_{SG}	rate constant for char steam gasification reaction, $\text{s}^{-1} \text{atm}^{-1}$
M_C	molecular weight of carbon (C), $\frac{\text{kg}}{\text{kmol}}$
n	reaction order, dimensionless
P_i	partial pressure of component i, atm
P_{O_2}	partial pressure of O_2 , atm
P_{H_2O}	partial pressure of H_2O , atm

R	gas constant 8.314×10^{-3} , $\frac{\text{kJ}}{\text{mol K}}$
r_c	total reaction rate of carbon (C) by char combustion and steam gasification reaction, $\frac{\text{kmol}}{\text{m}^3 \text{ s}}$
T_g	gasification temperature, K
X_{CO}	conversion of carbon (C) for char combustion reaction, dimensionless
X_{SG}	conversion of carbon (C) for char steam gasification reaction, dimensionless
Y_c	volume fraction of carbon (C) in solid, dimensionless
ρ_c	density of carbon (C), $\frac{\text{kg}}{\text{m}^3}$
ε_s	volume fraction of solid in bed, dimensionless

CHAPTER I

INTRODUCTION

1.1 Background

The fossil fuels (oil, coal, and natural gas) are the major sources of energy and raw material for petro-chemical industries in the world. These energy sources were used approximately 83 percentages of all energy consumption in Thailand 2010 as shown in Fig. 1 (Astalavista, 2013). However, the production of the fossil fuels is less than the consumption of the fossil fuels in Thailand, and hence, the amount of the imported fossil fuels can be shown in Fig. 2 (Astalavista, 2013). Moreover, usages of fossil fuels release carbon dioxide into the atmosphere which led to increased concerns about global warming issue as described in Fig. 3 (Enviromental risks, 2015 cited in Geographypods).

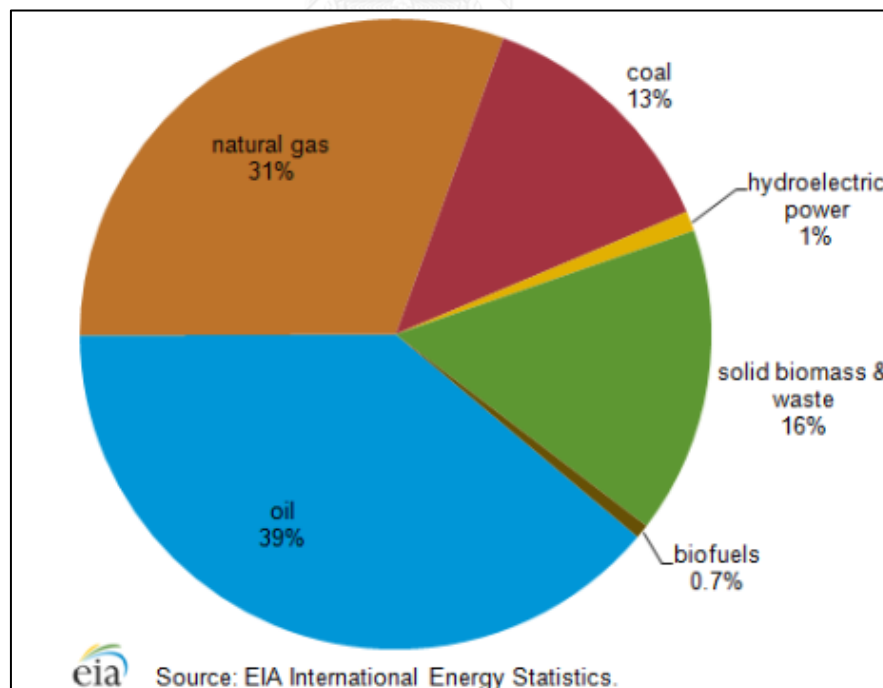


Fig. 1 Total energy consumption in Thailand in 2010 (Astalavista, 2013)

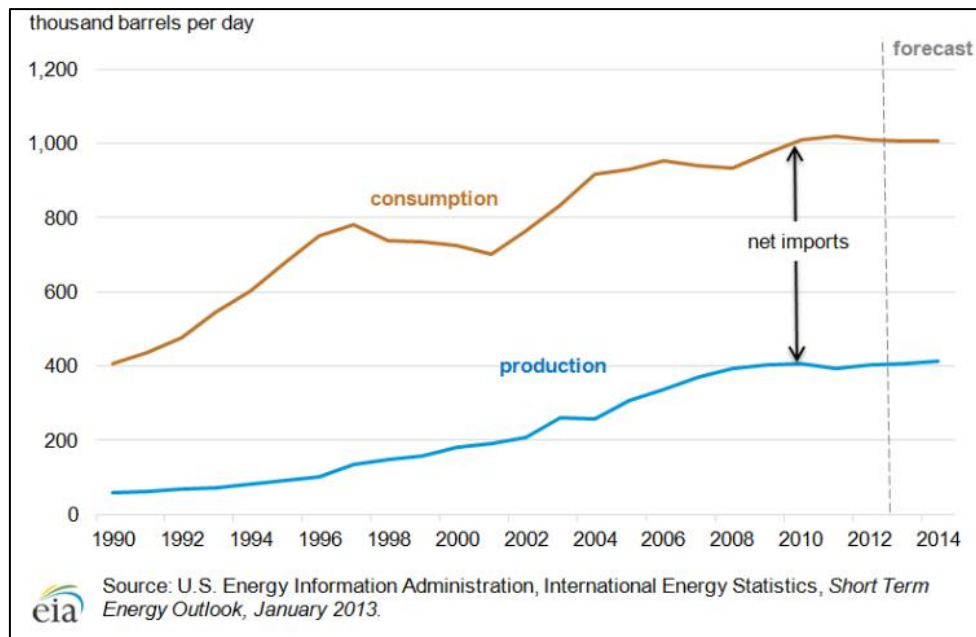


Fig. 2 Comparison between fossil fuels consumption and production in Thailand
(Astalavista, 2013)

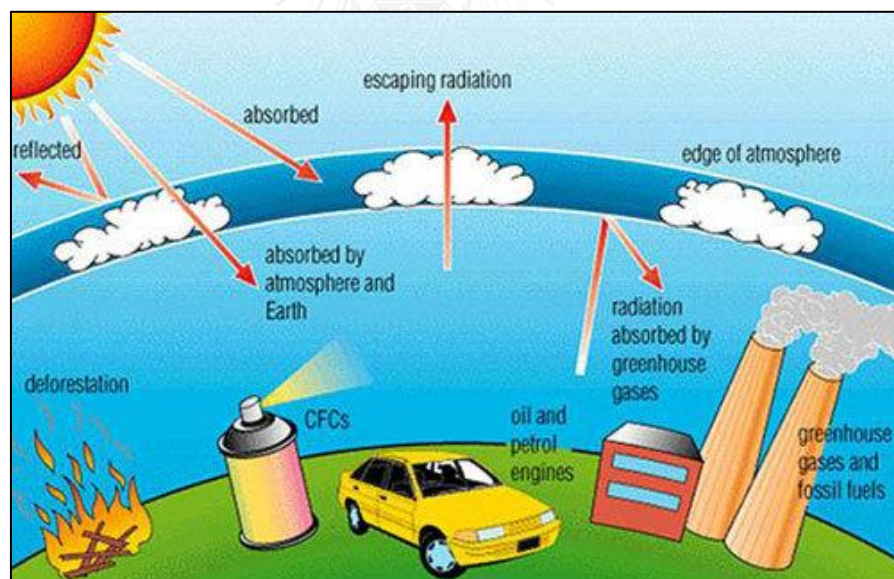


Fig. 3 The global climate change by carbon dioxide gas releasing
(Environmental risks, 2015 cited in Geographypods)

With the above mentioned situations, biomass is considered to be one of most interesting renewable energy sources. Biomass integrates solar energy and carbon dioxide into chemical energy in the form of carbohydrates via photosynthesis

reaction. The additional advantage of biomass is the carbon dioxide neutral process because the carbon dioxide which is released during combustion can be captured by the photosynthesis. The types of biomass fuels are various such as agricultural and forestry residues, woods, byproducts from processing of biological materials, and organic parts of municipal and sludge wastes (Kumar et al., 2009). Therefore, the physical and chemical properties of biomass used in gasification process are the factors that need to be considered as shown in Table 1 – 2 (Sharma & Kar, 2015).

Table 1 Relationship between the physical properties of biomass and process consideration (Sharma & Kar, 2015)

Physical properties of biomass	Process consideration
Moisture content	Storage, dry-matter losses
Volatiles	Thermal decomposition, combustion technology
Ash content	Dust emission, ash manipulation
Fixed carbon	Combustion technology
Calorific/ Heating value	Fuel utilization, plant design
Ash melting	Safety, process control
Fungi	Health risks
Bulk density	Logistics
Particle density, heat capacity, conductivity	Thermal decomposition
Dimension, shape	Conveying, drying, bridging, combustion technology

Table 2 Relationship between the chemical components of biomass and process consideration (Sharma & Kar, 2015)

Chemical components of biomass	Process consideration
Carbon (C)	Heating value
Hydrogen (H)	Heating value
Oxygen (O)	Heating value
Nitrogen (N)	NO _x , N ₂ O emissions
Chloride (Cl)	HCl, PCDD/F emissions, corrosion
Sulfur (S)	SO _x emissions, corrosion
Fluorine (F)	HF emissions, corrosion
Potassium (K)	Corrosion, ash melting
Sodium (Na)	Corrosion, ash melting
Magnesium (Mg)	Ash melting, utilization
Calcium (Ca)	Ash melting, utilization
Phosphorus (P)	Ash utilization
Heavy metals	Emission, ash melting

Two main ways of converting biomass energy (solid fuel) into biofuels and bio-power are biochemical conversion and thermochemical conversion processes. Biochemical conversions convert the biomass into liquid or gaseous fuels by fermentation or anaerobic digestion. Fermentation of the biomass (starch and cellulose) produces primarily ethanol. Anaerobic digestion leads to the production of gaseous fuel primarily containing methane. Thermochemical conversion technologies include combustion, gasification, and pyrolysis. The combustion of biomass is the most direct and technically easiest process but the overall efficiency of generating heat from biomass energy is low. The high combustion temperatures generate more NO_x and other emissions as shown in Table 3 (Breault, 2010). Gasification has many

advantages over combustion. The low heating value of biomass can be used with gasification. Moreover, the gasification process can convert biomass into the electricity and transportation fuels.

Table 3 The contrast between Combustion & Gasification (Breault, 2010)

Topic	Combustion	Gasification
Chemical process	Full oxidation	Partial oxidation
Chemical environment	Excess oxygen (air)-oxidizing	Oxygen-starved-reducing
Primary product	Heat (e.g., steam)	Syngas (CO & H ₂)
Downstream products	Electric power	Electric power, pure H ₂ , liquid fuels, chemicals
Current application	Dominates coal-fired power generator worldwide	Mostly chemicals and fuels, power generation demonstrated
Efficiency	35 – 37 (HHV)	39 – 42 (HHV)
Emissions	~NSPS	~1/10 NSPS
Capital cost	\$1,000 – 1,150/kW	Competitive
Maturity/ risk	High experience/ low risk	Reliability needs improvement

There are many studies of steam gasification processes. The examples of studies are atmospheric fluidized bed combustor processes (Douglas & Young, 1991), biomass gasification in fluidized bed reactor (Nikoo & Mahinpey, 2008), steam blown dual fluidized bed gasification (Doherty et al., 2013), biomass supercritical water gasification process (Nathapol, 2012), and bubbling fluidized bed gasification (Beheshti et al., 2015). Most studies have been focused on the effect of operating conditions in gasification process without concerning about the energy optimization in steam gasification process. The reason why energy optimization should be taken into account is because it can give the most suitable operating conditions that result

in the minimum quantity of energy required in process. This discovered benefit is very important and interesting, so the energy optimization of steam gasification process has been selected to study in this research.

The method of energy optimization used in this study is to find the energy self-sufficient condition. At this condition, all reaction heats are exchanged among each other inside the gasifier, and the energy input from the environment equals to zero. The energy self-sufficient condition of gasification process can be performed by adjusting three operating parameters (gasification temperature, equivalence ratio, and steam-to-biomass ratio). Therefore, this study was started with designing and creating the simulation model. Input process parameters that input in the simulation model were referred from the study of Nikoo & Mahinpey (2008). The simulation model had given good agreement with the experimental data from the referenced study. Consequently, the simulation model was used to study energy optimization.

1.2 Objective

The objective of this study was to optimize the required energy used in a steam gasification process by considering three operating parameters (gasification temperature, equivalence ratio and steam-to-biomass ratio) in order to achieve an energy self-sufficient condition.

1.3 Scope of research

The scope of this research could be listed as follows:

1.3.1 To develop simulation models of a steam gasification process which give good agreement with the experimental data

1.3.2 To analyze the effect of operating condition on the product gas compositions (hydrogen, carbon dioxide, carbon monoxide, and methane) and carbon conversion efficiency; the operating conditions were varied as below:

- Gasification temperature: 700 – 900 °C
- Equivalence ratio (ER): 0.19 – 0.27

- Steam-to-biomass ratio (SB): 0 – 4.04

1.3.3 To optimize the external required energy of the steam gasification process in the following steps

- Design the simulation test run with several batches in order to find an energy self-sufficient condition; equivalence ratio and steam-to-biomass ratio were varied in range of 0 – 0.31 and 0 – 4.49 respectively
- Run the simulation model in order to find the most suitable gasification temperature in each batch
- Demonstrate surface area of the selected operating condition by 3-D graphical diagram
- Optimize the surface area of the selected operating condition that the result of carbon conversion efficiency and carbon dioxide oxide gas composition under the criteria the carbon conversion efficiency must be more than 70 percentages, and carbon dioxide oxide gas was lower than 20 volumatic percentages

1.4 Expected benefits

To obtain the optimized operating region of three operating parameters (gasification temperature, equivalence ratio and steam-to-biomass ratio) which result in the minimum required energy.

CHAPTER II

LITERATURE REVIEW

A review of literature which is related to this work had been performed in order to gain the background knowledge of research scope, and in order to discover interesting issues and problems in the area that have been identified by other researchers. Moreover, the literature review was a procedure for data collecting in terms of research theory, methodology, and basic assumption that were used in this research. Many previous studies were concerned with the chemical process for steam gasification, in which the details were demonstrated in the following sections. To provide the better understanding of the details of the past researches and this work, some theories related to this research scope were explained in CHAPTER III and IV.

2.1 Biomass gasification process

At present, biomass gasification process is widely accepted as a popular technology to produce fuel gas for the application in steam turbine, gas turbine, boilers, and engine. In this chapter, the various aspects of biomass gasification process were reviewed, including biomass gasifier configurations and the effect of various operating parameters on the quality of product gas. Warnecke (2000) classified biomass gasifiers in to four categories which are based on the fluid and/or solid movement inside the reactor: (i) non-moving or self-moving feedstock, (ii) mechanically-moved feedstock (updraft gasifier, downdraft gasifier, and cross-draft gasifier), (iii) fluidically-moved feedstock (circulating fluidized bed (CFB) gasifier, bubbling fluidized bed (BFB) gasifier, and entrained-bed gasifier), and (iv) special reactors (cyclone gasifier and spouted bed gasifier). Among those above lists, updraft gasifier, downdraft gasifier, circulating fluidized bed (CFB), and bubbling fluidized bed (BFB) gasifier are widely used in the commercial market. Commercially, about 75 % of the gasifiers sold are downdraft gasifier, 20 % are fluidized bed gasifier, 2.5 % are updraft gasifier, and 2.5 % are of the other types (Knoef, 2000). The composition of

production gas varies widely and mostly depends on the gasifier type, feedstock type, feedstock pre-treatment, gasifying medium and operating parameters (gasification temperature, equivalence ratio and steam-to-biomass ratio). The characteristics of each gasifier type can be shown in Table 4 (Maurstad, 2005).

Table 4 Characteristics of different gasifier types (Maurstad, 2005)

Gasifier type	Fixed bed	Fluidized bed	Entrained flow
Outlet temperature	Low (425 – 600 °C)	Moderate (900 – 1050 °C)	High (1250 – 1600 °C)
Oxidant demands	Low	Moderate	High
Ash conditions	Dry ash or slagging	Dry ash or agglomerating	Slagging
Size of coal feed	6 – 50 mm	6 – 10 mm	< 0.1 mm
Acceptability of fines	Limited	Good	Unlimited
Other characteristics	Methane, tars and oils present in syngas	Low carbon conversion	Pure syngas, high carbon conversion

2.2 Steam gasification of biomass in fluidized bed reactor

Doherty et al. (2013) studied the effect of gasification temperature, biomass moisture, steam-to-biomass ratio, equivalence ratio, and air/steam supplying temperature on the composition of synthesis gas, heating value, and cold gas efficiency (CGE). A dual fluidized bed gasifier as known as the fast internally circulating fluidized bed (FICFB) gasifier was simulated with ASPEN PLUS. The simulation model was based on Gibbs free energy minimization and the restricted equilibrium method was applied by RGIBBS reactor. The gasification temperature and steam-to-biomass ratio were found to have strong influence on synthesis gas

composition and heating value. Biomass moisture had the most significant impact on cold gas efficiency (CGE).

The detailed process model was developed to simulate steam gasification of biomass in a bubbling fluidized bed (BFB) by ASPEN PLUS and dedicated FORTRAN subroutines (Beheshti et al., 2015). Effects on parameters (gasification temperature, steam-to-biomass ratio, equivalence ratio, and biomass particle size) on the composition of fuel gas were analyzed. The results showed that the high temperature was more favorable for production of useful synthesis gas (H_2 and CO) and hydrogen yield. Equivalence ratio was the most important factor in the process. The higher of equivalence ratio contributed to the higher carbon conversion, tar reforming, and gas yield. However, steam-to-biomass ratio was recognized as a key factor to produce more hydrogen rich gas but had a major effect on CO_2 formation.

Nikoo & Mahinpey (2008) studied the steam gasification of biomass in fluidized bed reactor by combination of kinetic reaction and hydrodynamic reaction with the equal volume of CSTR reactor. There were many chemical reactions occurred during pyrolysis and gasification steps such as combustion reaction, water gas reaction, water gas shift reaction, Boudouard reaction, etc. These chemical reaction could be consolidated to the combustion of char reaction and the steam gasification of char reaction. The combustion of char reaction consisted of the complete oxidation and the partial oxidation of carbon, the reaction gave product gases of carbon dioxide and carbon monoxide. The proportion of product gases depended upon the stoichiometric ratio of air and biomass. The steam gasification of char reaction consisted of water gas reaction and water gas shift reaction which gave product gases of carbon dioxide, carbon monoxide and hydrogen. The proportion of product gases depended upon the stoichiometric ratio of steam and biomass. The operation sets (gasification temperature, equivalence ratio, steam-to-biomass ratio, and biomass particle size) were varied in order to study their effects on the composition of product gases and carbon conversion efficiency. The experiment of fluidized bed gasifier was set up and compared the result with the simulation model. The results of varied temperature showed that the prediction of carbon dioxide, carbon monoxide and methane were conformed to the experimental results but the

prediction of hydrogen was not conformed. The temperature did not affect the hydrogen composition by simulation model while the higher temperature significantly increased hydrogen composition by experiment. The results of varied equivalence ratio showed that the prediction of hydrogen, carbon dioxide and carbon monoxide were conformed to the experimental results but the prediction of methane was not conformed. The equivalence ratio did not affect the methane composition by simulation model while the equivalence ratio decreased methane composition by experiment. The results of varied steam-to-biomass showed that the predictions of hydrogen and carbon monoxide were conformed to the experimental results but the prediction of carbon dioxide and Methane were not conformed. The steam-to-biomass ratio decreased carbon dioxide composition and did not affect to the methane composition by simulation model while the steam-to-biomass ratio increased carbon dioxide composition and decreased methane composition by experiment.

2.3 Kinetic model of char combustion and char gasification reactions

Lee et al. (1998) set the experiment to determine the kinetic reaction rate of coal gasification in a fluidized bed reactor. The char particles for the thermo-balance reactor were prepared by de-volatilization of Australian subbituminous coal. The coal was heated from room temperature to 900°C at the rate of 10°C per minute, and then maintained for 30 minutes at 900°C. The coal-particle diameters for the pyrolysis and gasification reactions were between 0.25 and 1.0 mm. The experiment varied the gasification temperature between 750 and 900 °C, coal feed rate between 0.76 and 2.23 kg/h, air/coal feed weight ratio between 1.5 and 3 and steam/coal feed weight ratio between 0.63 and 1.26. The activation energies and reaction-rate constants for the combustion and steam-gasification reactions were determined from an Arrhenius plot using data obtained with the thermos-balance reactor. Kinetic values were calculated by using the rate of conversion with time at different reaction temperatures on the basis of the shrinking-core model. Finally, the activation energies and reaction-rate constants of steam gasification reaction were found to be -

19,544 K, and $6,474.7 \text{ s}^{-1} \text{ atm}^{-1}$. But the activation energies and reaction-rate constants of combustion reaction were depended on the reaction control step where $k_i = 75,785 \text{ s}^{-1} \text{ atm}^{-1}$ and $E_i/R = 13,523 \text{ K}$ for the chemical-reaction-controlled regime; $k_i = 0.44 \text{ s}^{-1} \text{ atm}^{-1}$ and $E_i/R = 3342.4 \text{ K}$ for the pore-diffusion-controlled regime; and $k_i = 0.046 \text{ s}^{-1} \text{ atm}^{-1}$ and $E_i/R = 1166 \text{ K}$ for the gas-film-diffusion-controlled regime (Lee et al., 1998).

2.4 The energy self-sufficient condition of supercritical water gasification

Nathapol (2012) investigated the performance of the auto-thermal biomass gasification process in supercritical water by developing simulation model to compare with the experimental data. The prediction model was run under an energy self-sufficient condition, or minimum of the external energy demand. The total energy demand could be calculated by the summation of the energy demand in biomass decomposition process, biomass gasification process, and adjusting temperature process. The energy self-sufficient condition could be achieved by controlling the equivalence ratio at 0.04 for water hyacinth and 0.39 for rice straw with the operation conditions (gasification temperature at $700 \text{ }^\circ\text{C}$, and steam-to-biomass ratio at 0.1 and 1 for water hyacinth and rice straw, respectively).

CHAPTER III

THEORY AND METHODOLOGY

3.1 Basic of gasification process

The degradation of its molecular structure will be taken place after biomass is fed to the gasification process in order to produce a fuel and/or synthesis gases. The ability to totally convert a carbonaceous material largely depends on the extent of degradation that can be brought about. Typically, the complete conversion of biomass to product gas or liquid is impossible in a single step. In general, there are five different routes available for the degradation of a solid carbonaceous material that can be shown in Fig. 4 (Latif, 1999).

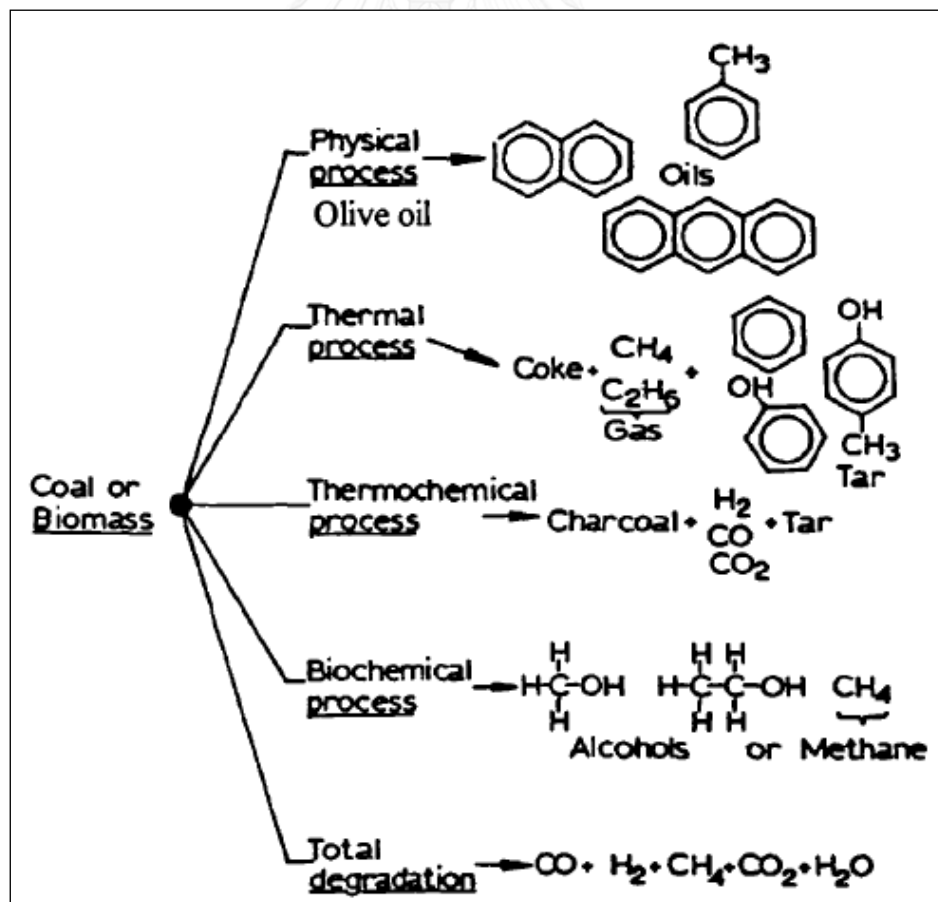


Fig. 4 Alternative Biomass Degradation Route Paths (Latif, 1999)

As mentioned above, there are several conversion route paths available such as thermal process (combustion), thermochemical process (gasification, pyrolysis) and biological process (anaerobic digestion, fermentation to ethanol). At present, thermal and thermochemical processes are more efficient and easier to operate since they result in almost complete conversion.

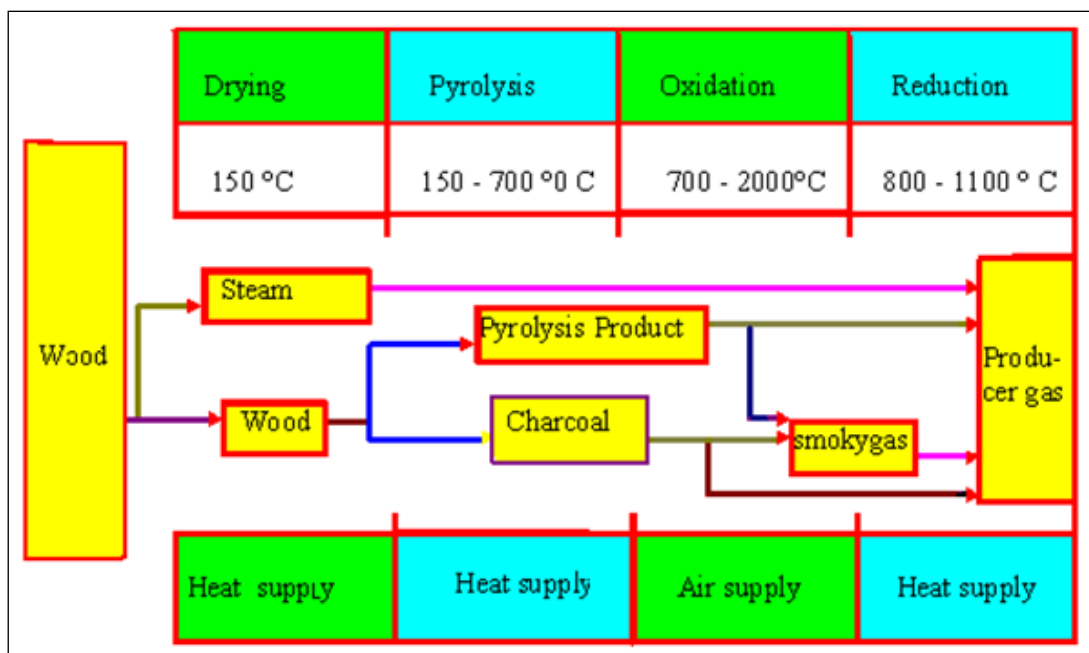


Fig. 5 The conversion of biomass into produced gases by thermochemical process (Biomass Gasification Technology and Utilization, 2015 cited in University of Flensburg)

A typical thermochemical process (gasification, pyrolysis) generally follows the chemical operation zones on the schematic illustration as shown in Fig. 5 (Biomass Gasification Technology and Utilization, 2015 cited in University of Flensburg).

- a) Preheating and drying
- b) Pyrolysis (De-volatilization)
- c) Combustion (Oxidation)
- d) Reduction (Char gasification)

Although these zones are frequently modeled in series but there is no sharp boundary between them. The biomass feedstock is firstly heated (dried) to remove some moisture out, and then it undergoes with pyrolysis step to be decomposed at high temperature. The products of pyrolysis step (i.e., solid, liquid and gas) react among themselves as well as with the gasifying medium to form the final gasification product. The chemical reactions that happened during pyrolysis step and gasification step can be basically presented in Table 5 (Latif, 1999).

Table 5 Basic reactions in gasification of carbonaceous materials (Latif, 1999)

		$\Delta H_{25^{\circ}\text{C}}$ (kJ/mol)
Pyrolysis		
(1) $4\text{C}_n\text{H}_m \rightarrow m\text{CH}_4 + (4n-m)\text{C}$	Pyrolysis reaction	Exothermic
Combustion		
(2) $\text{C} + 0.5\text{O}_2 \rightarrow \text{CO}$	Partial combustion reaction	- 111
(3) $\text{C} + \text{O}_2 \rightarrow \text{CO}_2$	Total combustion reaction	-394
Reduction		
(4) $\text{C} + \text{CO}_2 \rightarrow 2\text{CO}$	Boudouard reaction	+172
(5) $\text{C} + \text{H}_2\text{O} \rightarrow \text{H}_2 + \text{CO}$	Steam-carbon reaction	+131
(6) $\text{C} + 2\text{H}_2 \rightarrow \text{CH}_4$	Hydrogasification	-74.8
(7) $\text{CO} + \text{H}_2\text{O} \rightarrow \text{H}_2 + \text{CO}_2$	Water-gas-shift reaction	-41.2
(8) $\text{CO} + 3\text{H}_2 \rightarrow \text{CH}_4 + \text{H}_2\text{O}$	Methanation reaction	-206

Gasifier is the reactor that used for thermochemical process. There are many different designs of gasifiers which are mentioned by Warnecke (2000) in Chapter II. The chemical operation zones inside the gasifier can be shown in Fig. 6 (Marek, 2012).

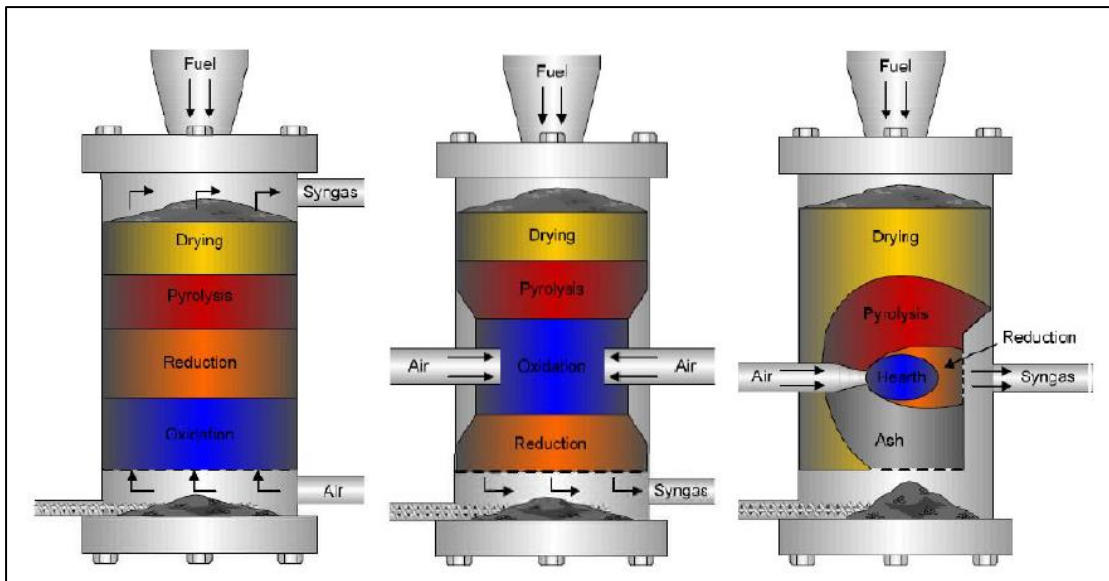


Fig. 6 Different types of fixed bed gasifiers, from the left: updraft, downdraft and cross draft (Marek, 2012)

3.2 Fluidized bed gasifier

The operation of fixed bed gasifiers is influenced by the morphological, physical and chemical properties of biomass. The problems which are commonly encountered for these gasifiers are lack of bunker flow, slugging and extreme pressure drop over the gasifier. Fluidized bed gasifier has been introduced to remove the problems and it is illustrated schematically in Fig.7 (Wood gas as engine fuel, 2015 cited in FAO Corporate Document Repository).

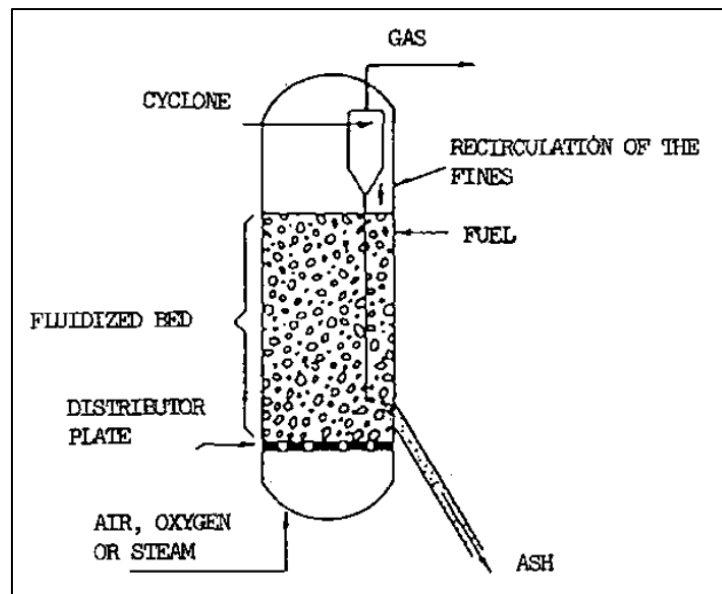


Fig. 7 Typical fluidized bed gasifier

(Wood gas as engine fuel, 2015 cited in FAO Corporate Document Repository)

Air is blown through a bed of solid biomass at a sufficient velocity to keep it at a suspension state. The biomass are introduced at the bottom of the reactor, very quickly mixed with the bed material and almost instantaneously heated up to the bed temperature. As a result of this treatment the pyrolysis of biomass is very fast, resulting in a component mix with a relatively large amount of gaseous materials. Further gasification and tar-conversion reactions occur in the gas phase. Most systems are equipped with an internal cyclone in order to minimize char blow-out as much as possible. Ash particles are also carried over the top of the reactor and have to be removed from the gas stream.

3.3 Effect of biomass feedstock on gasification process

3.3.1 Volatile matter

Biomass with high volatile matter is more reactive. It produces less char and is easy to make high gas conversion. Biomass feedstock generally contains high amount of volatile matter although it is very difficult to clean-up the gasifier because of high tar content (Mohit, 2011).

3.3.2 Ash

The ash content does not decide the product gas composition but it does have a profound impact on the practical operation of the gasifier. It is an unavoidable parameter which needs to be removed in either solid or liquid form depending upon the design of the gasifiers, the temperature profile, and the melting point of ash produced (Mohit, 2011).

3.3.3 Moisture

The moisture content is a decisive factor for the gasification process since high moisture content of the fuels can lead to the lower temperature inside the gasifier which can hinder the kinetics of gasification reactions. Therefore the feedstock should have an optimal moisture content of 5 - 10 % weight (Mohit, 2011).

3.4 Kinetic reaction

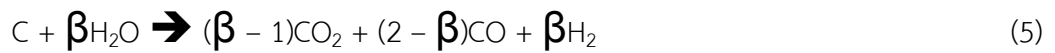
The gasification process begins with pyrolysis zone, then continues with volatile combustion zone and char gasification zone, respectively, as following reactions occur:

Combustion reaction (Lee et al., 1998):



Steam gasification reaction (Matsui et al., 1985):





α is a mechanism factor which is experimentally varied between 0.5 and 1 for partial combustion reaction. The reaction (5) is the combination of reaction (2), (3) and (4). Experimentally (Matsui et al., 1985), β can be determined to be in the range of 1.1 – 1.5 when the operating temperature is in the range of 750 – 900 °C. For this study, the values of α and β are selected to be to obtain the best agreement with experimental data at 0.7 and 1.3, respectively, The reaction rate equations according to the mentioned reactions can be defined as these equations.

$$\frac{dX_{\text{CO}}}{dt} = k_{\text{CO}} \exp\left(\frac{-E_{\text{CO}}}{RT_g}\right) P_{\text{O}_2}^n (1 - X_{\text{CO}})^{\frac{2}{3}} \quad (6)$$

$$\frac{dX_{\text{SG}}}{dt} = k_{\text{SG}} \exp\left(\frac{-E_{\text{SG}}}{RT_g}\right) P_{\text{H}_2\text{O}}^n (1 - X_{\text{SG}})^{\frac{2}{3}} \quad (7)$$

$$r_{\text{C}} = \left(\frac{dX_{\text{CO}}}{dt} + \frac{dX_{\text{SG}}}{dt} \right) \times \frac{\rho_{\text{C}} \varepsilon_{\text{S}} Y_{\text{C}}}{M_{\text{C}}} \quad (8)$$

The carbon conversion can be separately calculated with char combustion reaction as equation (6) and char steam gasification reaction as equation (7). The total reaction rate of carbon will be calculated as per equation (8). For atmospheric gasification, the steam partial pressure is in the range of 0.25 – 0.8 atm, the parameter n can be equal to 1 according to the study by Kasaoka et al. (1985). The kinetic parameter can be shown in Table 6 (Lee et al., 1998).

Table 6 Kinetic parameters of biomass gasification (Lee et al., 1998)

	E/R (K)	k (s ⁻¹ atm ⁻¹)
Combustion		
- The chemical-reaction-controlled regime	13,523	75,785
- The pore-diffusion-controlled regime	3,342.4	0.44
- The gas-film-diffusion-controlled regime	1,166	0.046
Steam gasification	19,544	6,474.7

3.5 Design information of steam gasification process

3.5.1 Equivalence ratio (ER)

It is defined as the ratio of actual air fuel ratio to the stoichiometric air fuel ratio. An excessive low value of ER (ER<0.2) results in several problems including incomplete gasification, excessive char formation and low heating value of product gas. On the other hand, the excessive high value of ER (ER>0.4) may result in formation of complete combustion (CO₂) rather than CO and H₂ which are the desired product gases.

$$ER = \frac{\text{weight of oxygen (air)/weight of dry biomass}}{\text{stoichiometric of oxygen (air)/biomass}} \quad (9)$$

3.5.2 Steam-to-biomass ratio (SB)

It is defined as the mass flow rate ratio of steam to biomass dry basis.

$$SB = \frac{\text{weight of steam}}{\text{weight of dry biomass}} \quad (10)$$

3.5.3 Carbon conversion efficiency

It is the ratio of the consumed carbon weight in gasification process to carbon feed weight.

$$\text{Carbon conversion efficiency} = 1 - \frac{(\text{total rate of carbon})_{\text{outlet stream}}}{(\text{total rate of carbon})_{\text{feed stream}}} \quad (11)$$

3.5.4 Operating condition

The operating condition is controlled based on the published data, simulation of biomass gasification in fluidized bed reactor using ASPEN PLUS by Nikoo & Mahinpey (2008) as shown in Table 7 (Nikoo & Mahinpey, 2008).



Table 7 Parameter inputs of simulation model (Nikoo & Mahinpey, 2008)

Biomass feedstock		
Proximate analysis		
- Moisture	wt.%	8
- Volatile matter	wt.% dry basis	82.29
- Fixed carbon	wt.% dry basis	17.16
- Ash	wt.% dry basis	0.55
Ultimate analysis		
- C	wt.% dry basis	50.54
- H	wt.% dry basis	7.08
- O	wt.% dry basis	41.11
- N	wt.% dry basis	0.15
- S	wt.% dry basis	0.57
- Ash	wt.% dry basis	0.55
Flow rate	kg/h	0.445-0.512
Air feedstock		
Temperature	°C	65
Flow rate	Nm ³ /h	0.5 – 0.7
Steam feedstock		
Temperature	°C	145
Flow rate	kg/h	0 – 1.8
Operating condition		
Temperature	°C	700 – 900
Pressure	atm	1

CHAPTER IV

SIMULATION MODEL

The process modeling is an effective instrument which can provide the opportunity to check the feasibility study of energy optimization of steam gasification process. ASPEN PLUS software has been selected because it is the powerful and adaptable tool for this simulation study. To ensure that the created process modelling can predict and analyze the outcome of a process, the validation with an experiment is widely used. In this study, the model will be validated with both experiment and simulation model results from Nikoo & Mahinpey (2008).

4.1 Basic assumptions for simulation of steam gasification process

- a) The simulation process is steady state
- b) The operation zone inside gasifier is isothermal condition
- c) The volatile products after de-volatilization of biomass mainly comprised of H_2 , CO, CO_2 , CH_4 and H_2O .
- d) Char is considered to have component of only carbon black and ash since the gasifier type is fluidized bed and the equivalence ratio is controlled in proper range
- e) Biomass de-volatilization is instantaneous in comparison to char gasification.
- f) The simulation is carried with power-law kinetics.
- g) The residence time for reactants is sufficiently high to reach the equilibrium of Gibbs free energy during pyrolysis reaction.

4.2 ASPEN PLUS modelling

The many operation steps of gasification process in fluidized bed reactor were separately considered in ASPEN PLUS simulation as biomass decomposition and volatile reactions in pyrolysis zone, char gasification in combustion and reduction

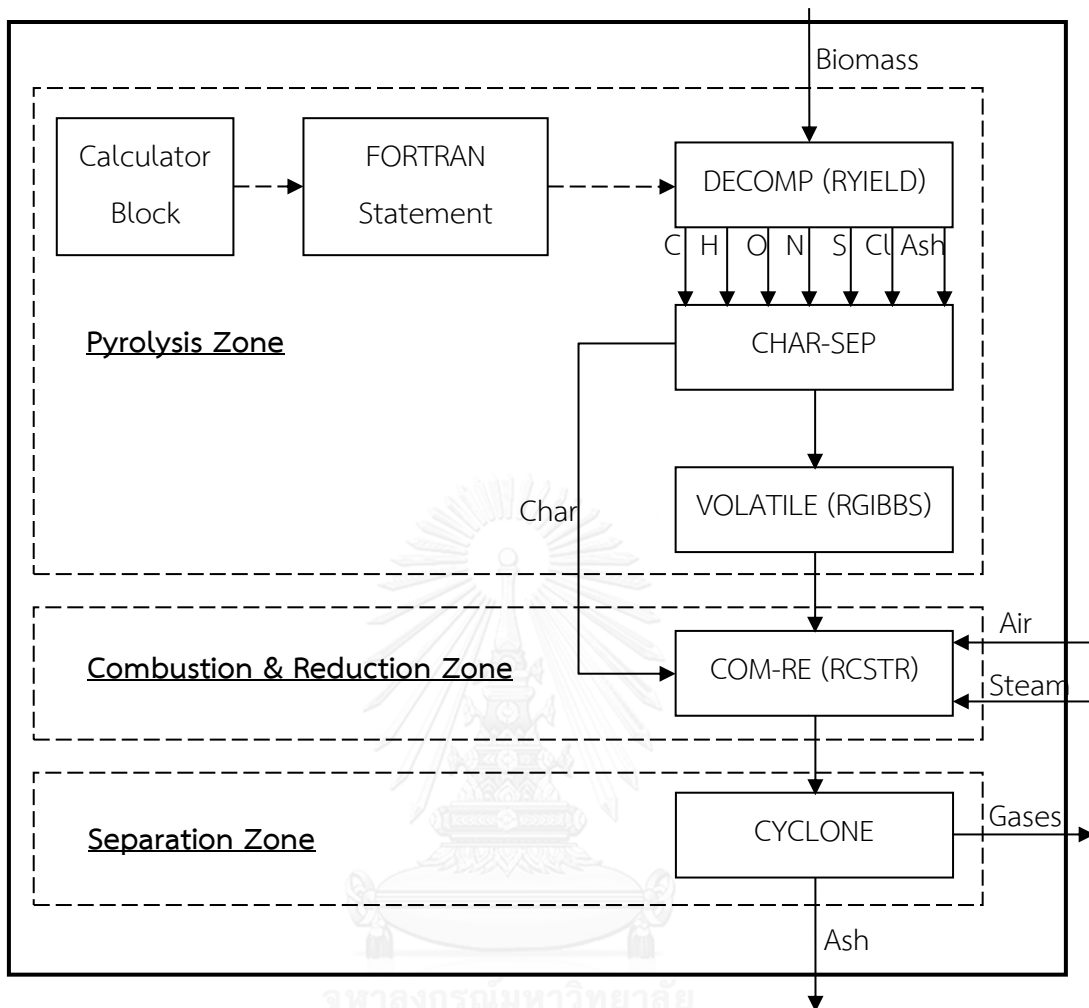


Fig. 9 Simulation calculation procedure of steam gasification process

4.2.1 Biomass decomposition

The ASPEN PLUS yield reactor, RYIELD, had been used to simulate the decomposition of the biomass feed stream. In this step, biomass was converted into its constituting components including carbon, hydrogen, oxygen, sulfur, nitrogen, and ash by specifying the yield distribution according to the biomass proximate and ultimate analysis.

The biomass had been input in the simulation program as unconventional component according to proximate and ultimate analysis properties. The operating temperature and pressure, production components

had been identified in reactor DECOMP. The production yield distribution could be calculated as shown in FORTRAN statement below.

C FACT IS THE FACTOR TO CONVERT THE ULTIMATE ANALYSIS TO A WET C BASIS.

$$\text{FACT} = (100 - \text{WATER}) / 100$$

$$\text{H2O} = \text{WATER} / 100$$

$$\text{ASH} = \text{ULT} (1) / 100 * \text{FACT}$$

$$\text{CARB} = \text{ULT} (2) / 100 * \text{FACT}$$

$$\text{H2} = \text{ULT} (3) / 100 * \text{FACT}$$

$$\text{N2} = \text{ULT} (4) / 100 * \text{FACT}$$

$$\text{CL2} = \text{ULT} (5) / 100 * \text{FACT}$$

$$\text{SULF} = \text{ULT} (6) / 100 * \text{FACT}$$

$$\text{O2} = \text{ULT} (7) / 100 * \text{FACT}$$

4.2.2 Volatile reaction

The ASPEN PLUS Gibbs reactor, RGIBBS, had been used for volatile combustion, in conformity with the assumption that volatile reactions followed the equilibrium of Gibbs free energy. Biomass consisted of mainly C, H, O, N, S, Cl, ash and moisture. Carbon partly constituted the gas phase, which took part in devolatilization, and the remaining carbon comprised part of the solid phase (char) and subsequently resulted in char gasification. A SEPARATION COLUMN model had been used to separate the volatile materials and solids.

The separation column CHAR-SEP can separate the solid phase of carbon with the assumption that char is considered as only components of carbon black and ash. The equation of char separation could be shown as below.

C FIXEDCARB IS THE SOLID COMBUSTIBLE RESIDUE THAT CONTAINED WITH CARBON. IT CAN BE CALCULATED BY %FC OF PROXIMATE ANALYSIS

$$\text{FIXDCARB} = \text{FC} / 100 * \text{FACT}$$

$$\text{CHAR} = \text{CARB} - \text{FIXDCARB}$$

The operating temperature and pressure, possible production components had been identified in reactor VOLATILE. This reactor calculated the composition of product with the assumption that the residence time for reactants was sufficiently high to reach the equilibrium of Gibbs free energy during pyrolysis reaction. The calculation equation of free Gibbs energy could be shown as equation (12) – (14).

$$\Delta G_i^o = -RT \ln(K) \quad (12)$$

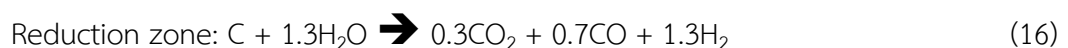
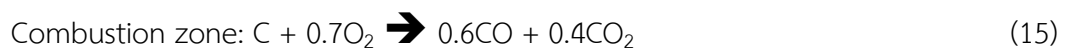
$$G_i = \Delta G_i^o + RT \ln(P_i) \quad (13)$$

$$\Delta G = \left(\sum_i^n G_i \right)_{\text{Product}} + \left(\sum_i^n G_i \right)_{\text{Reactant}} \quad (14)$$

4.2.3 Char gasification

The ASPEN PLUS CSTR reactor, RCSTR, performed char gasification by using reaction kinetics. The gasification reactor outlet was fed to gas-solid separation, the gases outlet from the separator were stabilized and purified, and the gas will be transferred by piping system to storage tank as fuel gas.

The operating temperature and pressure, reactor volume and reaction information had been identified in reactor COM-RE. This reactor calculated the composition of product with the assumption that the simulation was carried out with the power-law kinetics. The gas-film-diffusion-controlled regime of combustion reaction was selected to the input kinetic parameters. The stoichiometric reaction of combustion zone and reduction zone could be shown as per equation (15) – (16).



The reasons of reactor block selection were depended upon the limitation of reaction information which was available to input in to the simulation model. The reactor blocks that were used in this study could be shown in Table 8 (Aspen Technology, 2014).

Table 8 Reactor blocks description in the simulation (ASPEN PLUS Version 8.2, 2014)

Reactor block	Description
RYIELD	Models a reactor by specifying reaction yields of each component. This model is useful when reaction stoichiometry and kinetics are unknown and yield distribution data or correlations are available.
RGIBBS	Models single-phase chemical equilibrium, or simultaneous phase and chemical equilibrium by minimizing Gibbs free energy, subject to atom balance constraints. This model is useful when temperature and pressure are known and reaction stoichiometry is unknown.
RCSTR	Models a continuous-stirred tank reactor. This is useful when reaction kinetics are known. This model is useful when solids, such as char, are participating in the reactions.

4.3 Model validation

The simulation model results were validated with the experimental data by calculating the root mean square error of product gas compositions hydrogen, carbon dioxide, carbon monoxide, and methane. The root mean square error can be calculated according to below equations (17) – (18).

$$\text{Mean Square Error (MSE)} = \frac{1}{N} \sum_{i=1}^N \left(\frac{y_{ie} - y_{ip}}{y_{ie}} \right)^2 \quad (17)$$

$$\text{Root Mean Square Error (RMSE)} = \sqrt{\text{MSE}} \quad (18)$$

Table 9 The root mean square error of simulation model result

Set of operating condition	Result by	Root Mean Square Error (RMSE)			
		H ₂	CO ₂	CO	CH ₄
Gas composition versus temperature	Nikoo & Mahinpey	0.3606	0.3009	0.1044	0.2152
	Simulation	0.1541	0.1225	0.0498	0.2076
% Reduction		57.26	58.48	52.30	3.53
Gas composition versus ER	Nikoo & Mahinpey	0.1981	0.2308	0.0939	0.1997
	Simulation	0.0357	0.0496	0.0357	0.0567
% Reduction		81.99	78.51	61.98	71.61
Gas composition versus SB ratio	Nikoo & Mahinpey	0.2045	0.2382	0.1143	0.2712
	Simulation	0.0552	0.1030	0.0552	0.1496
% Reduction		73.01	56.76	51.71	44.84

The simulation model gave good agreement with the experimental data as shown in Table 9. The root mean square errors of all product gas compositions in simulation result in this study were less than the result of Nikoo & Mahinpey (2008).

4.4 The effect of gasification temperature

The simulation results of temperature effect were shown as Fig. 10 – 14. The temperature rise made the rate of reaction and H₂ proportion increased, whereas CO, CO₂, and CH₄ are decreased. The carbon conversion efficiency was affected by temperature rising as well; it was increased when temperature rise as the reaction rate constant of char combustion/gasification reactions followed Arrhenius equation which was directly proportional to temperature.

In addition, the result of simulation could also explain production of gas with type of reaction and reactor. H₂ was produced by steam gasification reaction in reactor COM-RE (RCSTR). CO was produced by both volatile combustion reaction in

reactor VOLATILE (RGIBBS) and char combustion reactions in reactor COM-RE (RCSTR), whereas CO_2 was only produced by char combustion reactions in reactor COM-RE (RCSTR). And, CH_4 was only produced by volatile combustion reaction in reactor VOLATILE (RGIBBS) with free Gibbs energy equilibrium.

However, the simulation results showed that the compositions of CO_2 and CH_4 gases were not similar to the experimental data when temperature was over than 800 °C. The higher temperature could increase the proportion of the complete combustion of char, α value might be increased to 0.75 – 0.8 to give the better result. The methanation reaction ($\text{C} + 2\text{H}_2 \rightarrow \text{CH}_4$) should be input to reactor COM-RE (RCSTR) in order to improve the composition of CH_4 especially at high temperature.

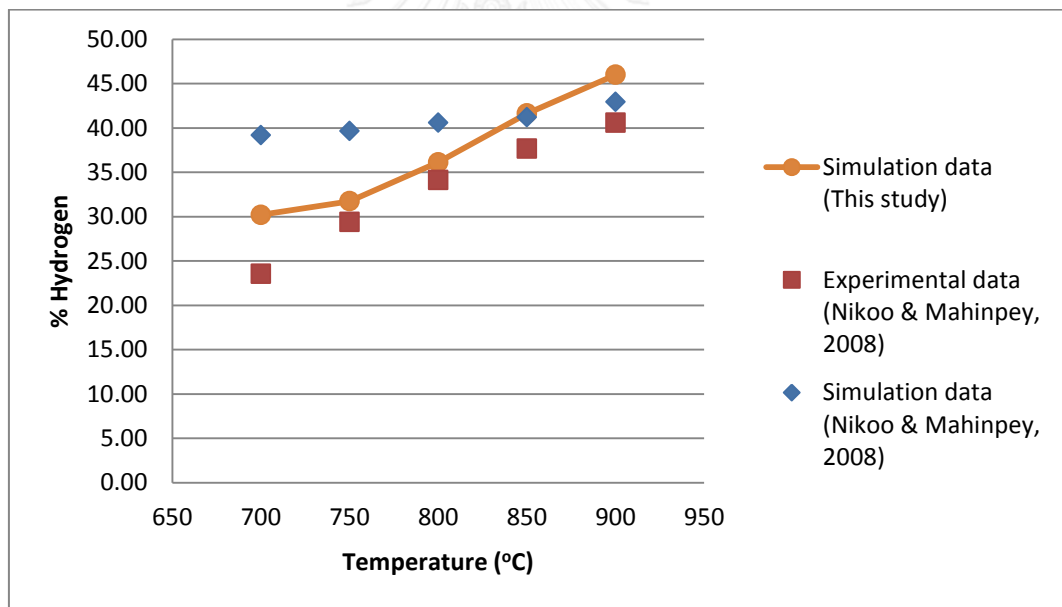


Fig. 10 Effect of temperature on hydrogen
(biomass: 0.445 kg/h, air: 0.5 Nm³/h, steam: 1.2 kg/h)

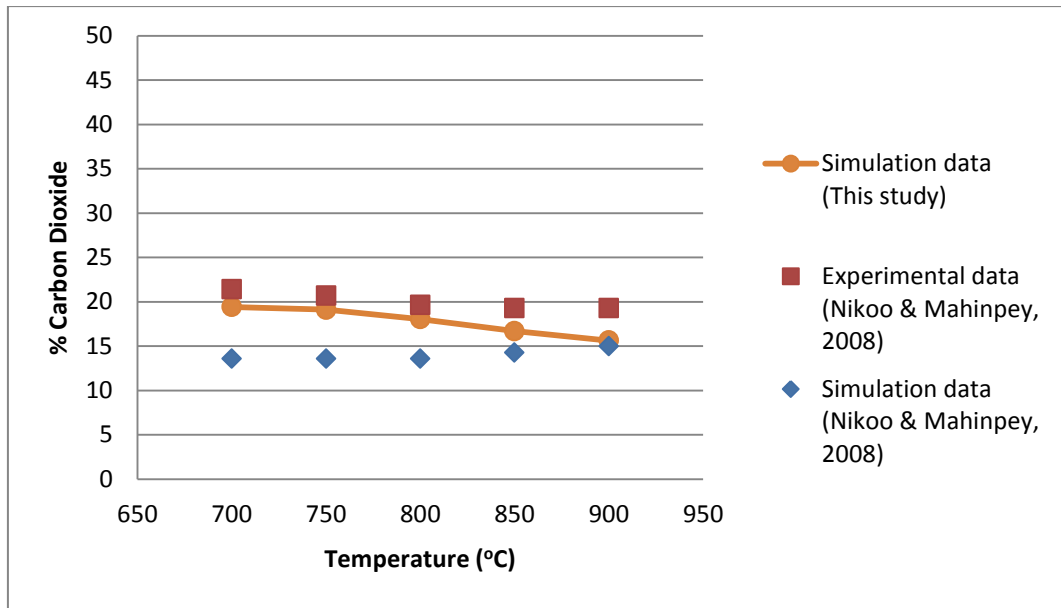


Fig. 11 Effect of temperature on carbon dioxide
(biomass: 0.445 kg/h, air: 0.5 Nm³/h, steam: 1.2 kg/h)

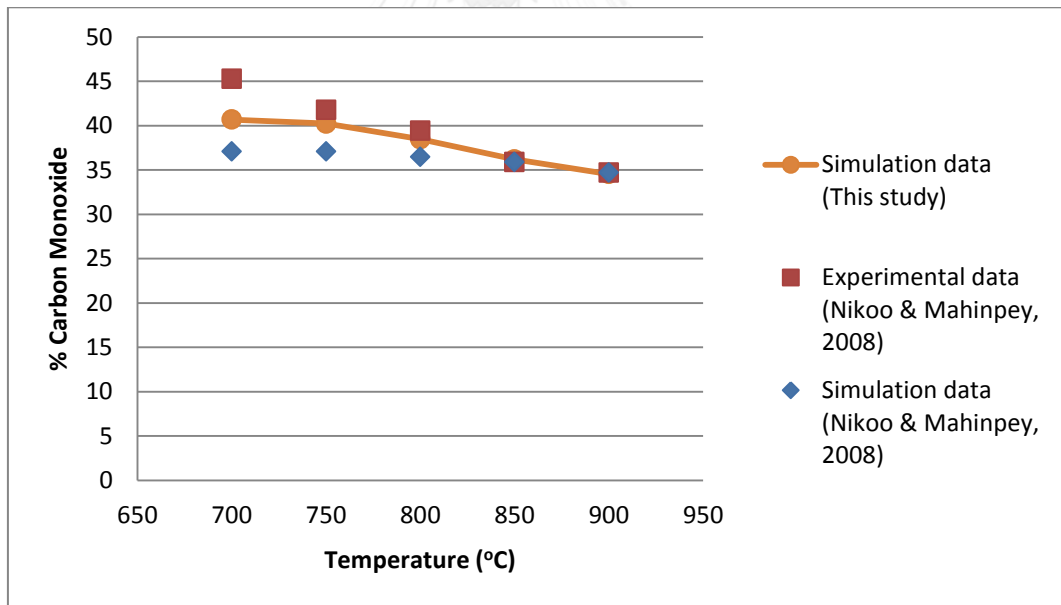


Fig. 12 Effect of temperature on carbon monoxide
(biomass: 0.445 kg/h, air: 0.5 Nm³/h, steam: 1.2 kg/h)

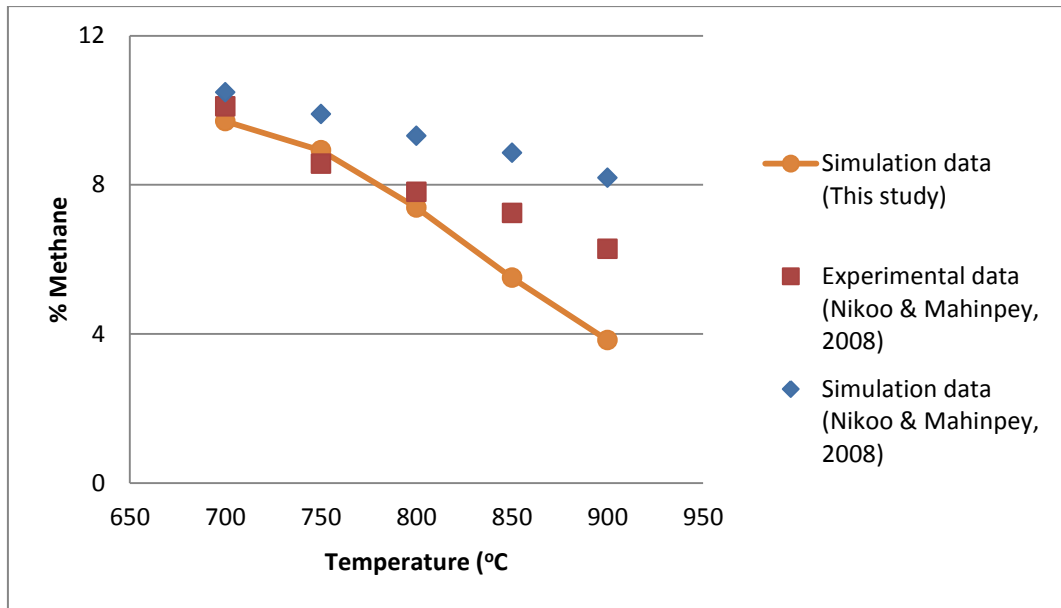


Fig. 13 Effect of temperature on methane
(biomass: 0.445 kg/h, air: 0.5 Nm³/h, steam: 1.2 kg/h)

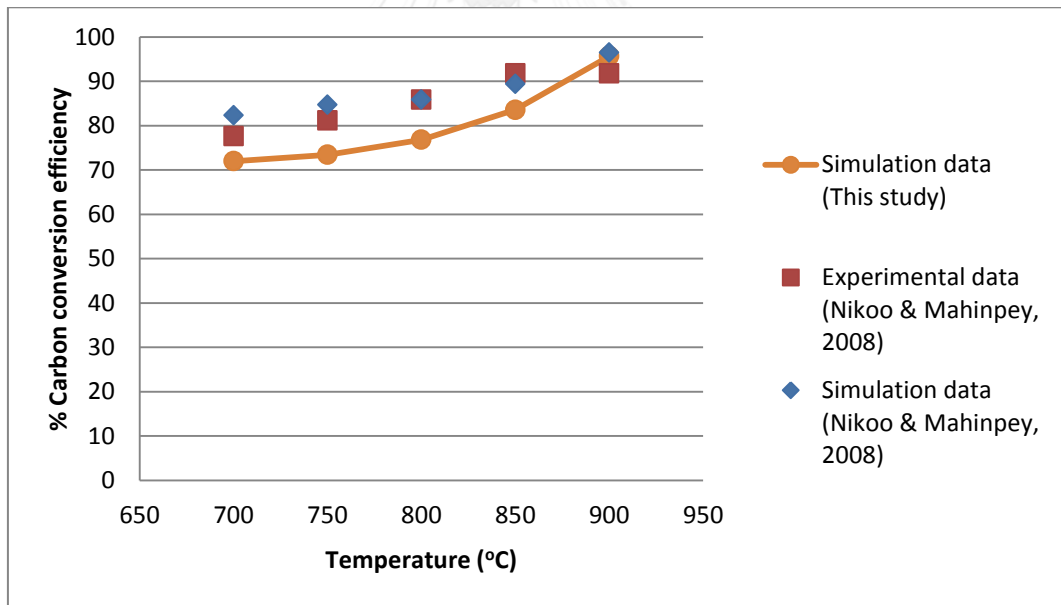


Fig. 14 Effect of temperature on % carbon conversion efficiency
(biomass: 0.445 kg/h, air: 0.5 Nm³/h, steam: 1.2 kg/h)

4.5 The effect of equivalence ratio (ER)

The simulation results of equivalence ratio effect were shown as Fig. 15 – 19. The increasing of equivalence ratio excited the reaction rate of char combustion reaction in RCSTR reactor. The carbon conversion efficiency was proportionally increased. Based on the stoichiometry of reaction (1), CO_2 was produced more than CO with the same amount of oxygen gas, therefore CO_2 and CO were increased. The increasing rate of CO_2 was more than the increasing rate of CO. CH_4 was not affected because the reaction rate of volatile combustion in RGIBBS reactor and char gasification in RCSTR reactor were not affected by the equivalence ratio. H_2 was decreased as the increasing of equivalence ratio reduced the reaction rate of char gasification by reducing the partial pressure of steam.

The simulation result showed that the carbon conversion efficiency was not similar to the experimental data when equivalence ratio was over than 0.23. The increase in equivalence ratio effectively increased the reaction rate of the combustion reaction of char, so the carbon conversion efficiency was also increased. However, the carbon conversion efficiency might be decreased in case that air was too much supplied. The biomass would be rapidly moved up to the gasifier before it could be completely reacted.

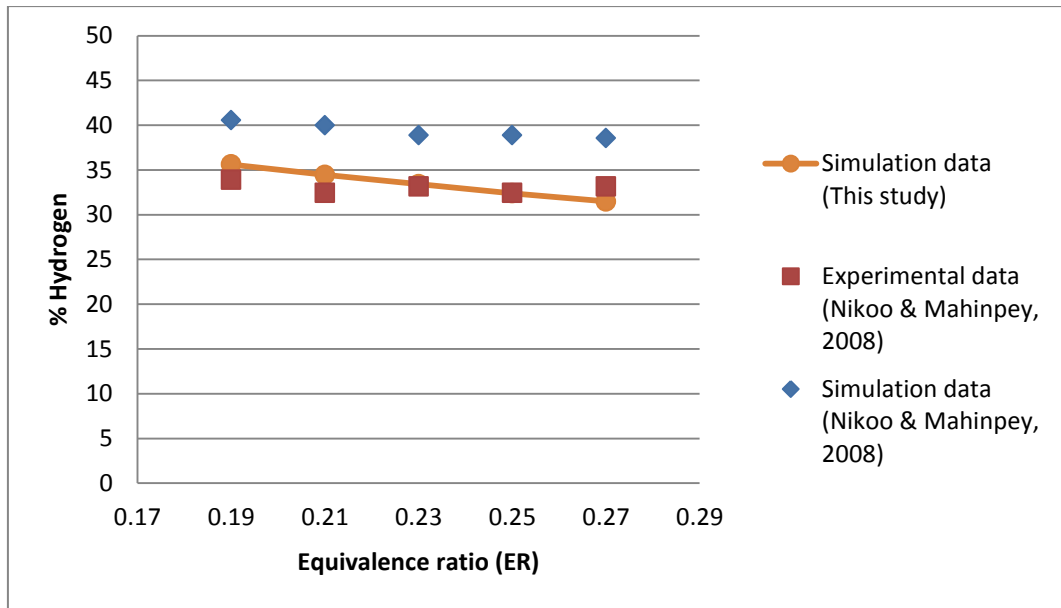


Fig. 15 Effect of equivalence ratio on hydrogen
(biomass: 0.512 kg/h, temperature: 800 °C, steam: 0.8 kg/h)

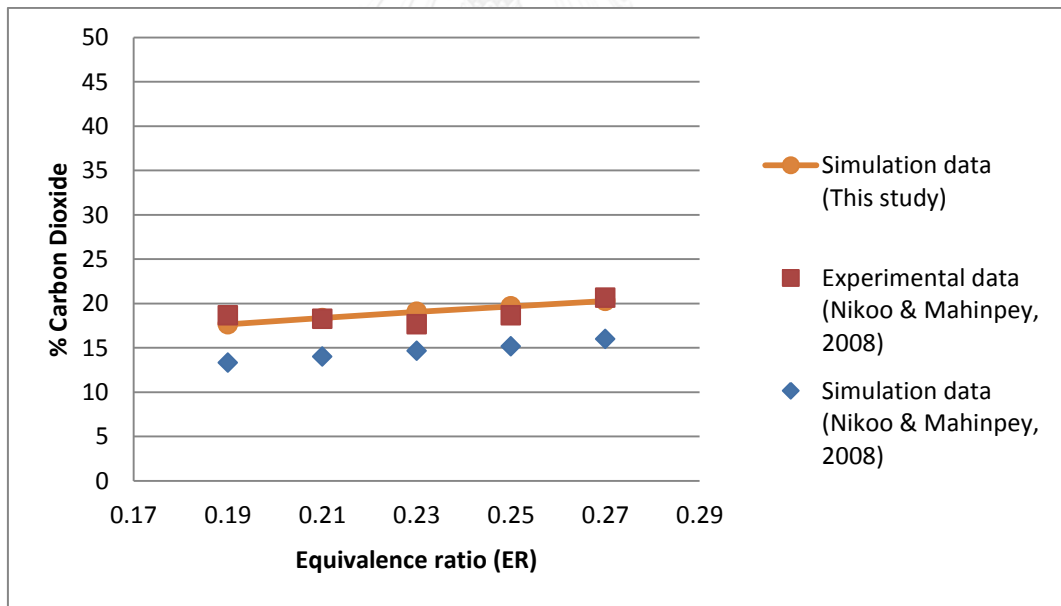


Fig. 16 Effect of equivalence ratio on carbon dioxide
(biomass: 0.512 kg/h, temperature: 800 °C, steam: 0.8 kg/h)

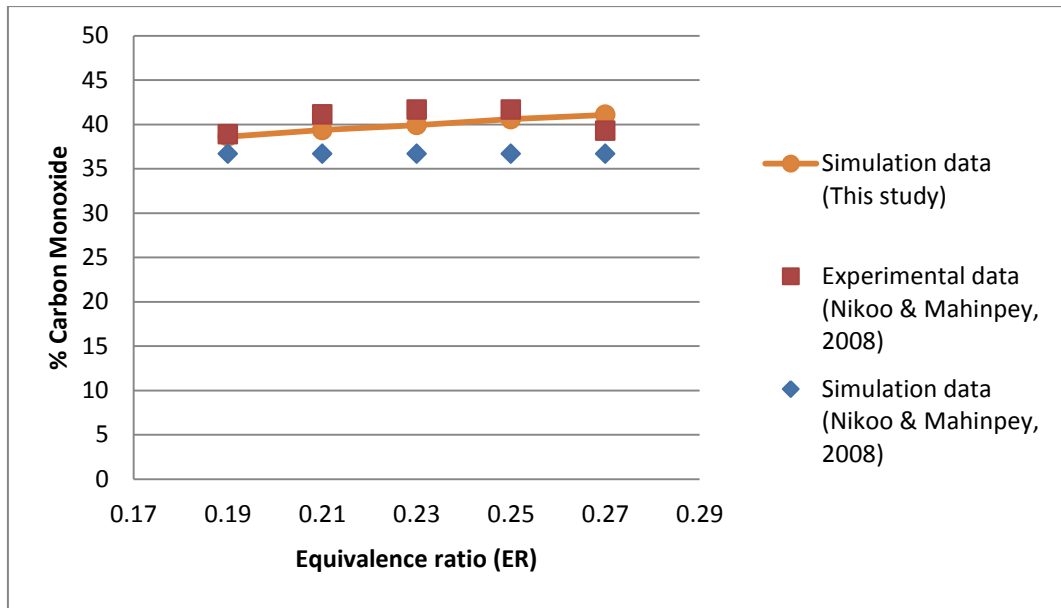


Fig. 17 Effect of equivalence ratio on carbon monoxide
(biomass: 0.512 kg/h, temperature: 800 °C, steam: 0.8 kg/h)

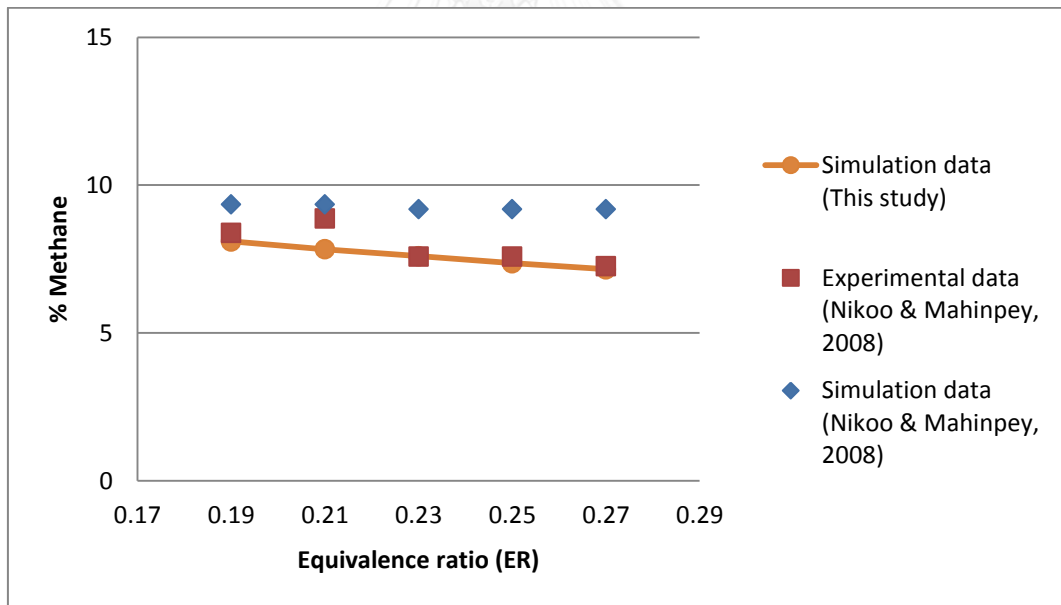


Fig. 18 Effect of equivalence ratio on methane
(biomass: 0.512 kg/h, temperature: 800 °C, steam: 0.8 kg/h)

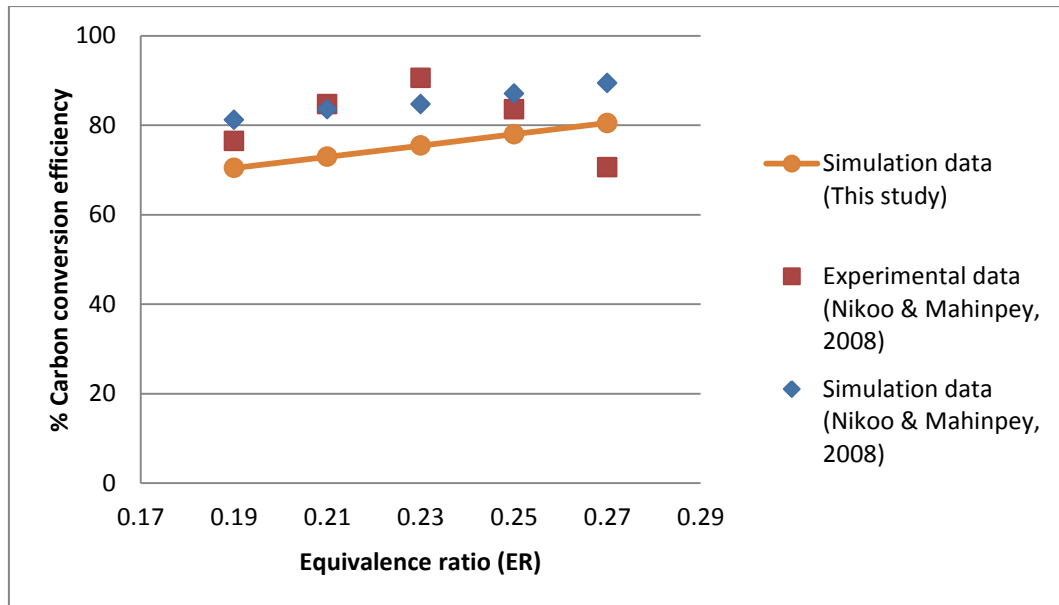


Fig. 19 Effect of equivalence ratio on % carbon conversion efficiency
(biomass: 0.512 kg/h, temperature: 800 °C, steam: 0.8 kg/h)

4.6 The effect of steam-to-biomass ratio (SB)

The simulation results of steam-to-biomass effect were shown as Fig. 20 – 24. The increasing of steam-to-biomass ratio excited the reaction rate of char gasification reaction in RCSTR reactor. This resulted increasing of carbon conversion efficiency. Refer to the stoichiometry of reaction (5), H₂ production was increased with increasing of reaction rate in comparison with CO and CO₂ that were not significantly affected. Because of the reaction rate of char combustion was much more than the reaction rate of char gasification. For CH₄, there was no effect as the reaction rate of volatile combustion in RIGBBS reactor and char gasification in RCSTR reactor were not affected by steam-to-biomass ratio.

The simulation result showed that the slope of carbon conversion efficiency by simulation result was less than the experimental data. The increase in steam-to-biomass ratio effectively increased the reaction rate of the gasification reaction of char, so the carbon conversion efficiency was also increased. However, the carbon

conversion efficiency might be decreased in case that steam was too much supplied. The moisture contain in biomass would be increased and obstructed the combustion reaction of char.

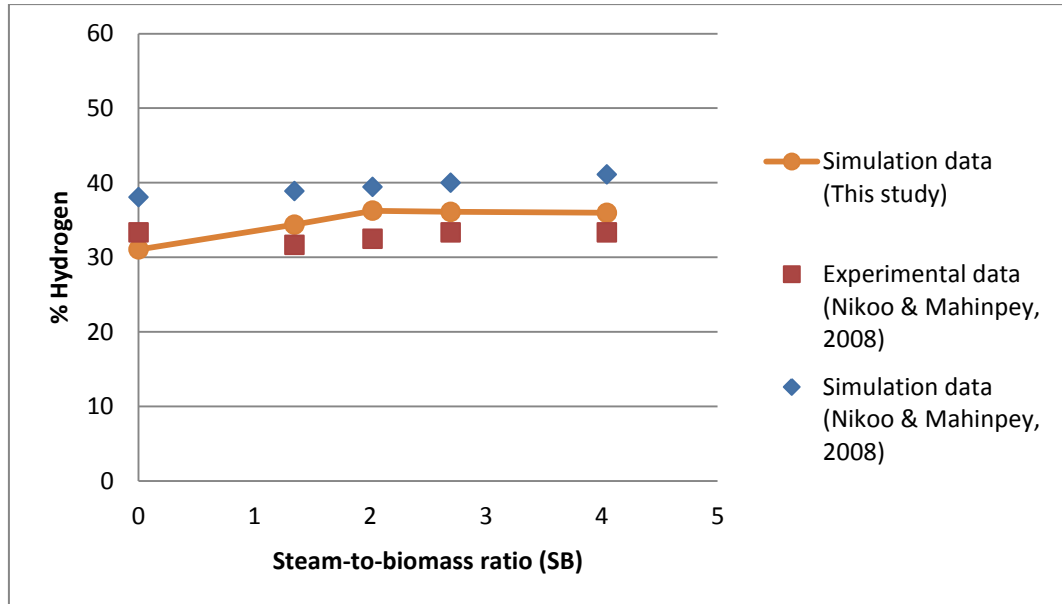


Fig. 20 Effect of steam-to-biomass ratio on hydrogen (biomass: 0.445 kg/h, temperature: 800 °C, air: 0.5 Nm³/h)

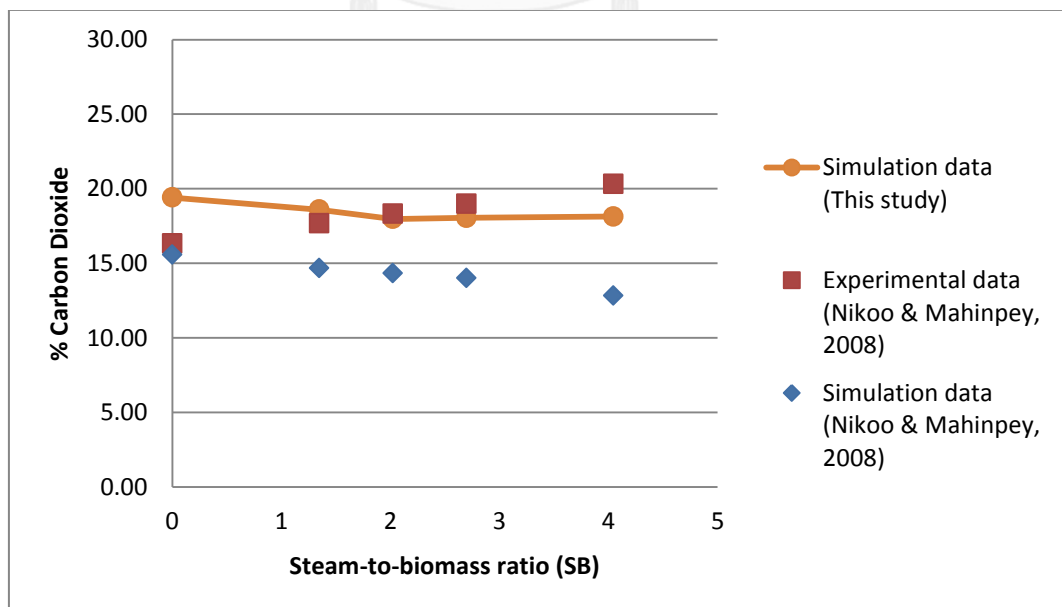


Fig. 21 Effect of steam-to-biomass ratio on carbon dioxide (biomass: 0.445 kg/h, temperature: 800 °C, air: 0.5 Nm³/h)

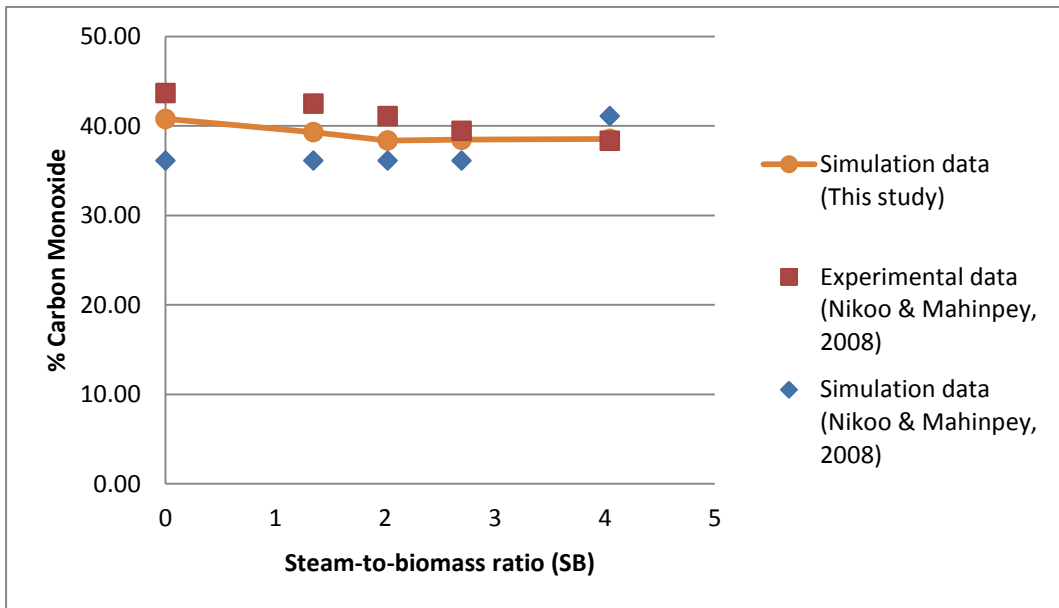


Fig. 22 Effect of steam-to-biomass ratio on carbon monoxide (biomass: 0.445 kg/h, temperature: 800 °C, air: 0.5 Nm³/h)

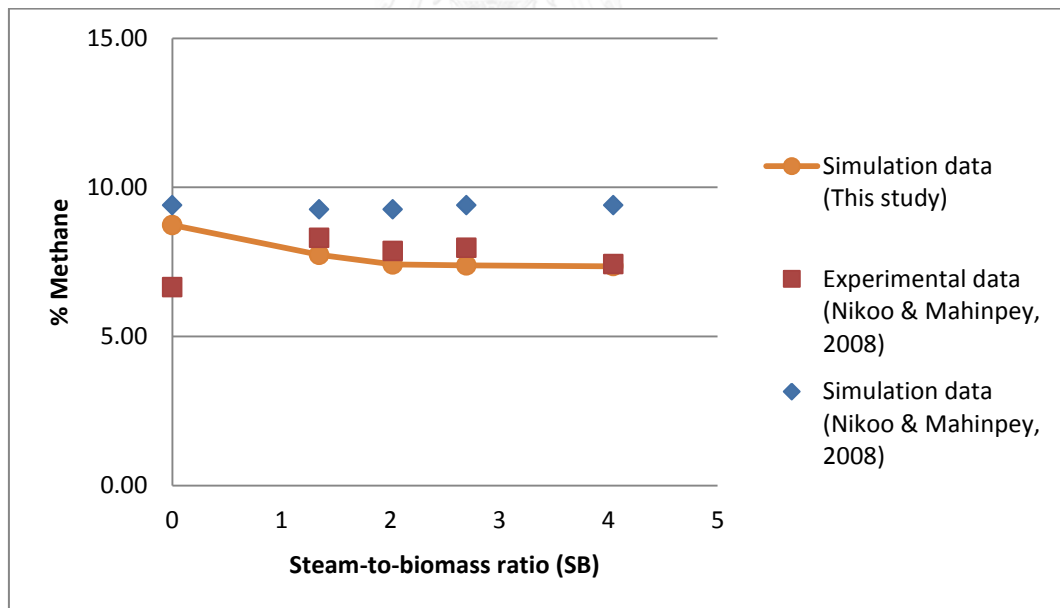


Fig. 23 Effect of steam-to-biomass ratio on methane (biomass: 0.445 kg/h, temperature: 800 °C, air: 0.5 Nm³/h)

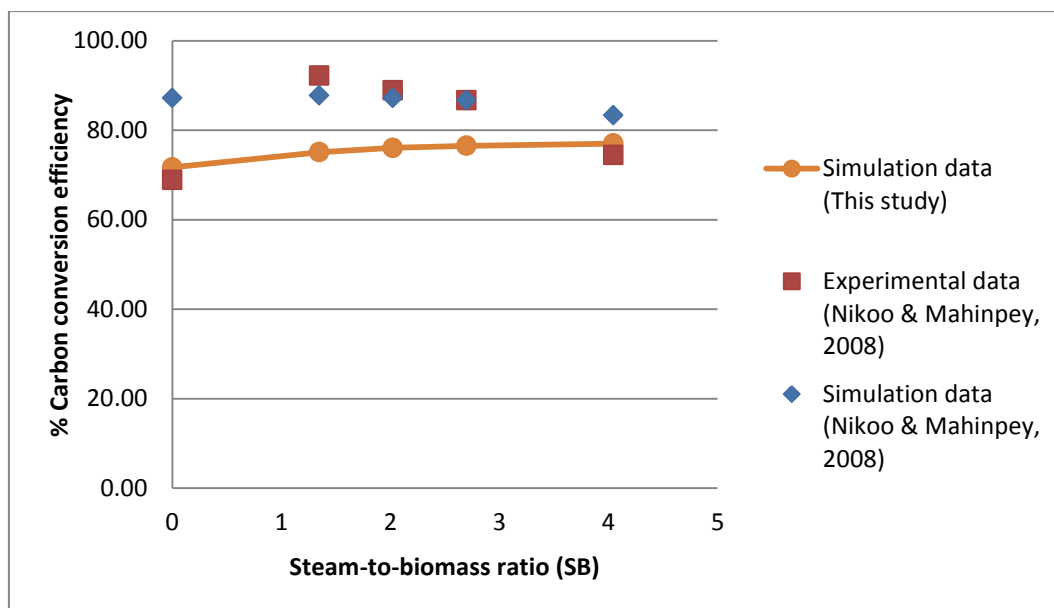


Fig. 24 Effect of steam-to-biomass ratio on % carbon conversion efficiency
(biomass: 0.445 kg/h, temperature: 800 °C, air: 0.5 Nm³/h)

CHAPTER V

THE EFFECT OF BIOMASS TYPE

Thailand is well-recognized as one of the lead exporters of agricultural and food products. This fact makes us realize that the more agricultural product produced, the more residue generated. At the same time, agricultural residues are the major source of biomass which has been used for fuel gases production and/or gases synthesis for decades. The various types of agricultural residues were used as biomass in Thailand, especially, non-plantation residue: (i) rice husk, (ii) rice straw, (iii) maize stalk, and (iv) sugar cane (Chaiyo & Deakhuntod, 2006).

Ubonwan and Jittawadee (2006) had studied the chemical properties of these agricultural residues to identify the proximate analysis and ultimate analysis results as per Table 10 – 11 (Chaiyo & Deakhuntod, 2006).

For this study, various types of biomass as mentioned were fed into simulation model instead of saw dust to study the outcome effect on each type of biomass under variation of temperature so as to recommend which one would be the most suitable to be used in a steam gasification process.

Table 10 The proximate analysis of Thai agricultural residues
(Chaiyo & Deakhuntod, 2006)

Properties	Rice husk	Rice straw	Maize stalk	Sugar cane
Moisture (wt.%)	6.65	6.71	8.42	7.94
Ash (wt.% dry basis)	20.47	25.25	5.73	8.35
Volatile matter (wt.% dry basis)	65.24	62.86	76.77	77.38
Fixed carbon (wt.% dry basis)	14.29	11.89	17.5	14.27

Table 11 The ultimate analysis of Thai agricultural residues
(Chaiyo & Deakhuntod, 2006)

Properties	Rice husk	Rice straw	Maize stalk	Sugar cane
C (wt.% dry basis)	0.32	0.55	1.29	0.8
H (wt.% dry basis)	32.36	41.03	43.95	44.57
O (wt.% dry basis)	4.03	4.62	5.77	5.86
N (wt.% dry basis)	0.08	0.09	0.01	0.01
S (wt.% dry basis)	42.74	28.46	43.25	40.41
Ash (wt.% dry basis)	20.47	25.25	5.73	8.35

5.1 Hydrogen component

The simulation result of temperature effect on hydrogen component was shown as Fig. 25. Temperature rise affected in direct proportional to H₂ gas percentage increase of all biomass types. However, rice husk produced H₂ gas less than rice straw, maize stalk, and sugar cane as its ultimate analysis property showed that it contained the least hydrogen element.

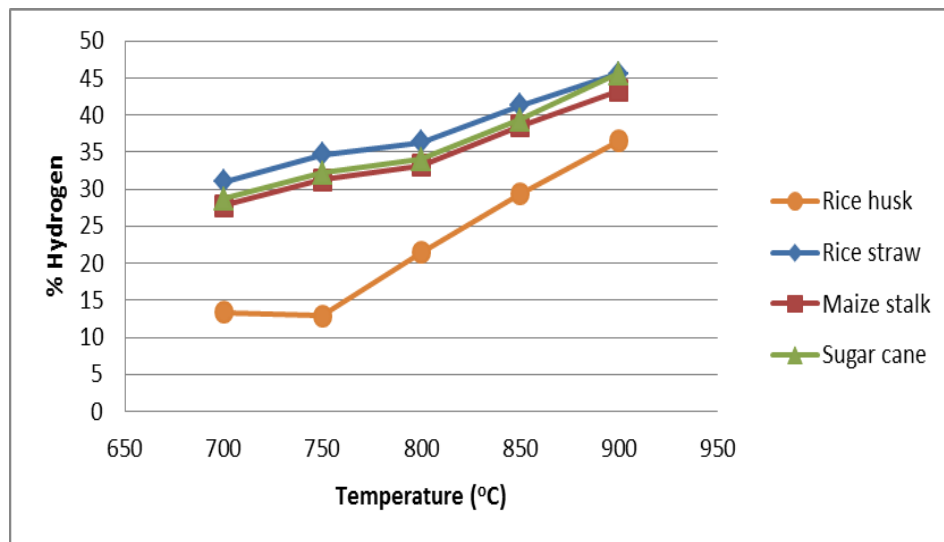


Fig. 25 Effect of temperature on hydrogen for various biomass types
(biomass: 0.445 kg/h, air: 0.5 Nm³/h, steam: 1.2 kg/h)



5.2 Carbon dioxide component

The simulation result of temperature effect on carbon dioxide component was shown as Fig. 26. Temperature rise affected in direct proportional to CO₂ gas percentage decrease of all biomass types. There was no difference in CO₂ gas production from any kind of biomasses.

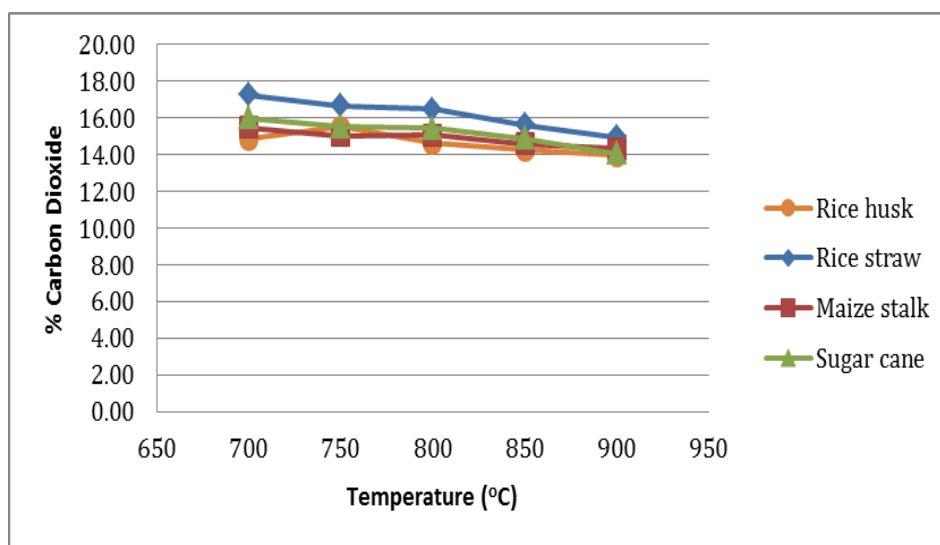


Fig. 26 Effect of temperature on carbon dioxide for various biomass types

(biomass: 0.445 kg/h, air: 0.5 Nm³/h, steam: 1.2 kg/h)

5.3 Carbon monoxide component

The simulation result of temperature effect on carbon monoxide component was shown as Fig. 27. Temperature rise affected in direct proportional to CO gas percentage decrease of all biomass types. However, rice husk produced CO gas more than rice straw, maize stalk, and sugar cane as its ultimate analysis property showed that it contained the greatest number of oxygen element.

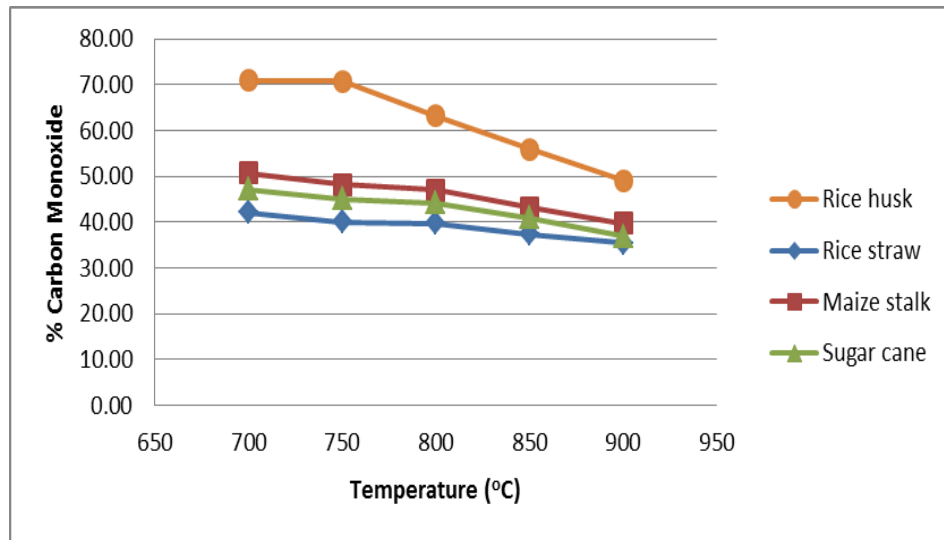


Fig. 27 Effect of temperature on carbon monoxide for various biomass types
(biomass: 0.445 kg/h, air: 0.5 Nm³/h, steam: 1.2 kg/h)

5.4 Methane component

The simulation result of temperature effect on methane component was shown as Fig. 28. Temperature rise affected in direct proportional to CH₄ gas percentage decrease of rice straw, maize stalk, and sugar cane, whereas CH₄ gas percentage of rice husk was constant. CH₄ gas production of sugar cane was less than other kinds of biomass due to high reaction rate of char combustion in RCSTR reactor.

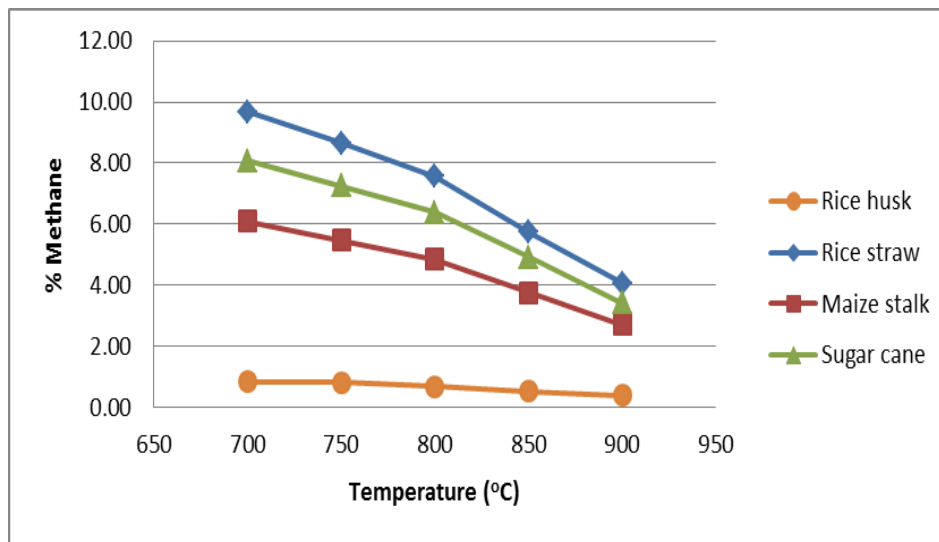


Fig. 28 Effect of temperature on methane for various biomass types
(biomass: 0.445 kg/h, air: 0.5 Nm³/h, steam: 1.2 kg/h)

5.5 Carbon conversion efficiency

The simulation result of temperature effect on carbon conversion efficiency was shown as Fig. 29. Temperature rise affected in direct proportional to carbon conversion efficiency increase of all biomasses. The carbon conversion efficiency was no significantly different between rice straw, maize stalk, and sugar cane. However, their efficiency was less than rice husk.

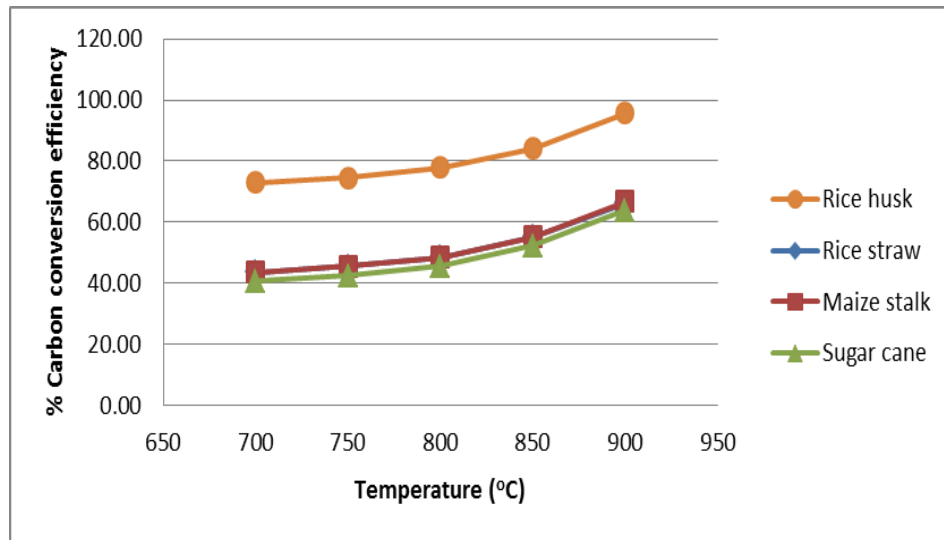


Fig. 29 Effect of temperature on % carbon conversion efficiency for various biomass types (biomass: 0.445 kg/h, air: 0.5 Nm³/h, steam: 1.2 kg/h)

The summary was that rice straw, maize stalk, and sugar cane had no difference in H₂, CO, and CO₂ gas production and carbon conversion efficiency whereas rice husk had the highest carbon conversion efficiency. However, CH₄ and H₂ gases production of rice husk were the least. Then, it could be concluded that rice straw was the most suitable biomass for steam gasification process because it produced CH₄ gas more than any kind of biomasses.

CHAPTER VI

HEAT OPTIMIZATION

This chapter described how to improve the energy efficiency of the steam gasification process. Fig. 30 showed the total required energy of steam gasification process which could be calculated by the summation of the required energy of all reactors (DECOMP, VOLATILE, and COM-RE) as showed as equation (19). In case that the total required energy from the environment was equal to zero, the gasification process could be operated without any required energy. This operating condition is called “the energy self-sufficient condition. The appropriate adjustment of operating parameters (gasification temperature, equivalence ratio, and steam-to-biomass ratio) was the key to achieve.

$$Q_{\text{gasifier (net)}} = Q_{\text{decomp}} + Q_{\text{volatile}} + Q_{\text{com-re}} \quad (19)$$

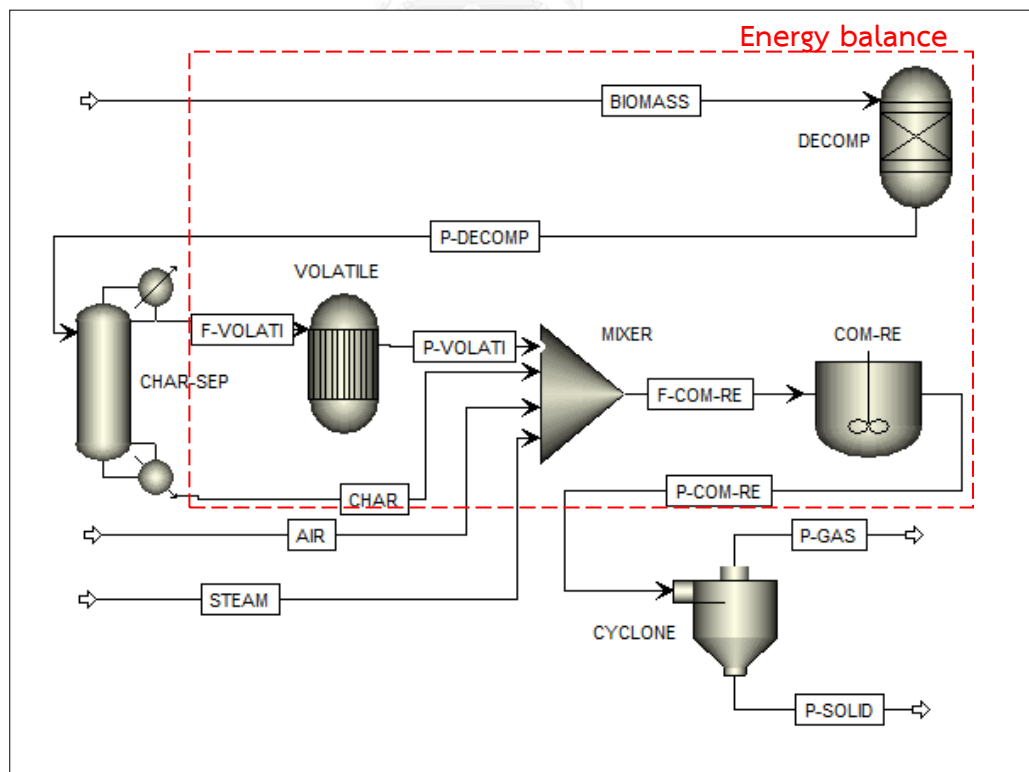


Fig. 30 The system of energy balance of steam gasification process in fluidized bed reactor

The trial and error of operating conditions had been selected as the technic in order to find the various sets of suitable operating parameter. The simulation test runs were separately set to forty-eight batches that would give enough results. Biomass was fed into the process at 0.445 kg/h. Air supply flow rate was varied from 0 to 0.7 Nm³/h, or the equivalence ratio was varied from 0 to 0.31. Steam supply flowrate was varied from 0 to 2 kg/h, or the steam-to-biomass ratio from 0 to 4.49. In each single batch, equivalence ratio and steam-to-biomass ratio were fixed to find the energy self-sufficient condition by adjusting the gasification temperature. The example of trial and error in 39th batch which fixed the equivalence ratio at 0.26 and steam-to-biomass ratio at 3.56 can be shown in Fig. 31. The increase in gasification temperature effectively raised the total required energy. The total required energy was zero when gasification temperature was 837 °C. Therefore, the optimum operating parameters of this batch were gasification temperature at 837 °C, equivalence ratio at 0.26, and steam-to-biomass ratio at 3.56.

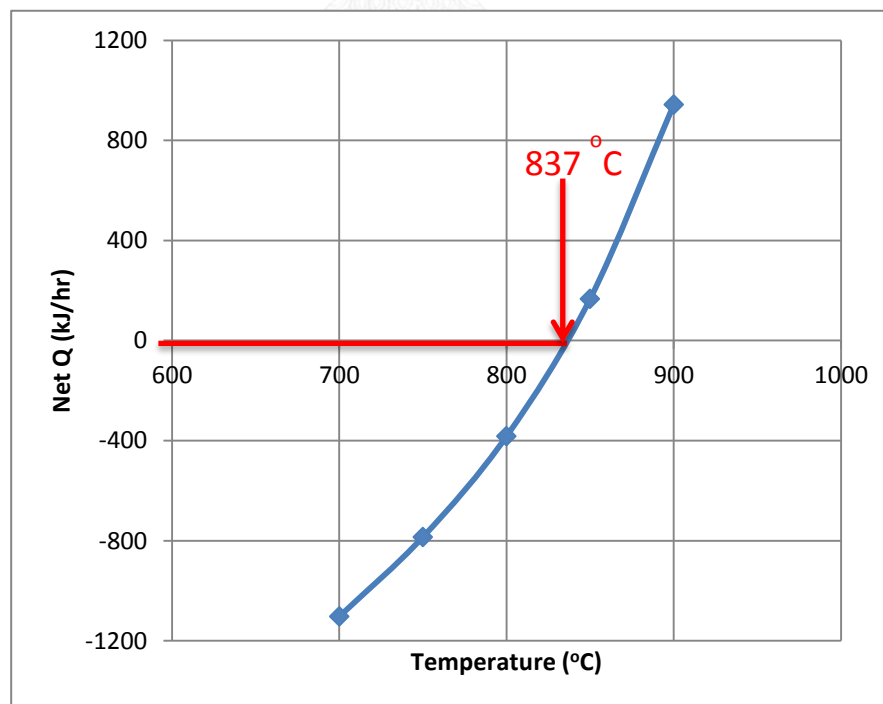


Fig. 31 The trial and error result of total required energy in 39th batch (biomass: 0.445 kg/h, air: 0.6 Nm³/h, steam: 1.6 kg/h)

After completion of the simulation test run, the 3-D plot graph among gasification temperature, equivalence ratio, and steam-to-biomass ratio could give the surface area of the energy self-sufficient condition as shown in Fig. 32.

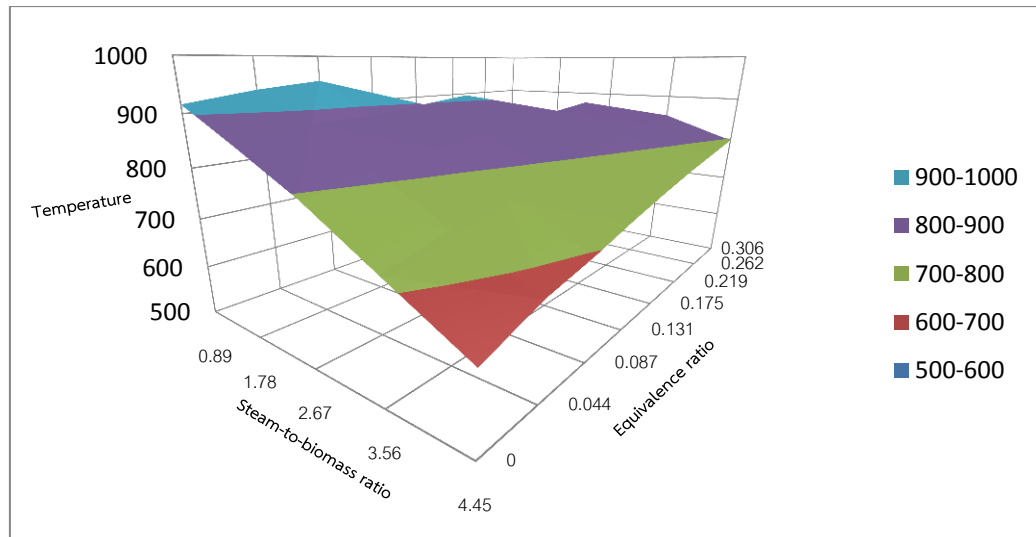


Fig. 32 The relationship of key parameters for the energy self-sufficient condition

The gas composition produced by the common gasifier types were given in Table 12 (Boerrigter & Rauch, 2006). The product distribution was depended on the conditions that used in the gasification, such as the gasification medium, gasifier design, residence time, etc. The average volumetric percentage of carbon dioxide is at 29 % for atmospheric circulating fluidized bed with steam/oxygen (ACFB). Refer to general property of fuel gas, the more amount of carbon dioxide decrease, the higher heating value of product gas would be. Then, the suitable criteria of gas composition to expand heating value, was the amount of carbon dioxide gas should be lower than 20 volumatic percentages and the carbon conversion efficiency shall be more than 70 percentages.

Table 12 The gas composition leaving common gasifiers, Atmospheric Circulating Fluidized Bed with steam/oxygen (ACFB), Pressurized Circulating Fluidized Bed with

steam/oxygen at 20 bara (PCFB) and Indirectly heated gasifier
(Boerrigter & Rauch, 2006)

Gasification process:		ACFB	PCFB	Indirect
Pressure [bara]:	Unit	1	20	
Gasification medium:		Steam/oxygen	Steam/oxygen	
H ₂	Vol-%	32	19	15 – 20
CO ₂	Vol-%	29	40	10 – 12
CO	Vol-%	27	20	40 – 43
CH ₄	Vol-%	8	15	15 – 17
N ₂	Vol-%	0	0	1 – 4
C ₂ +	Vol-%	3	5	5 – 6
Benzene	Vol-%	1	1	1
Tar	g/Nm ³	11	16	40



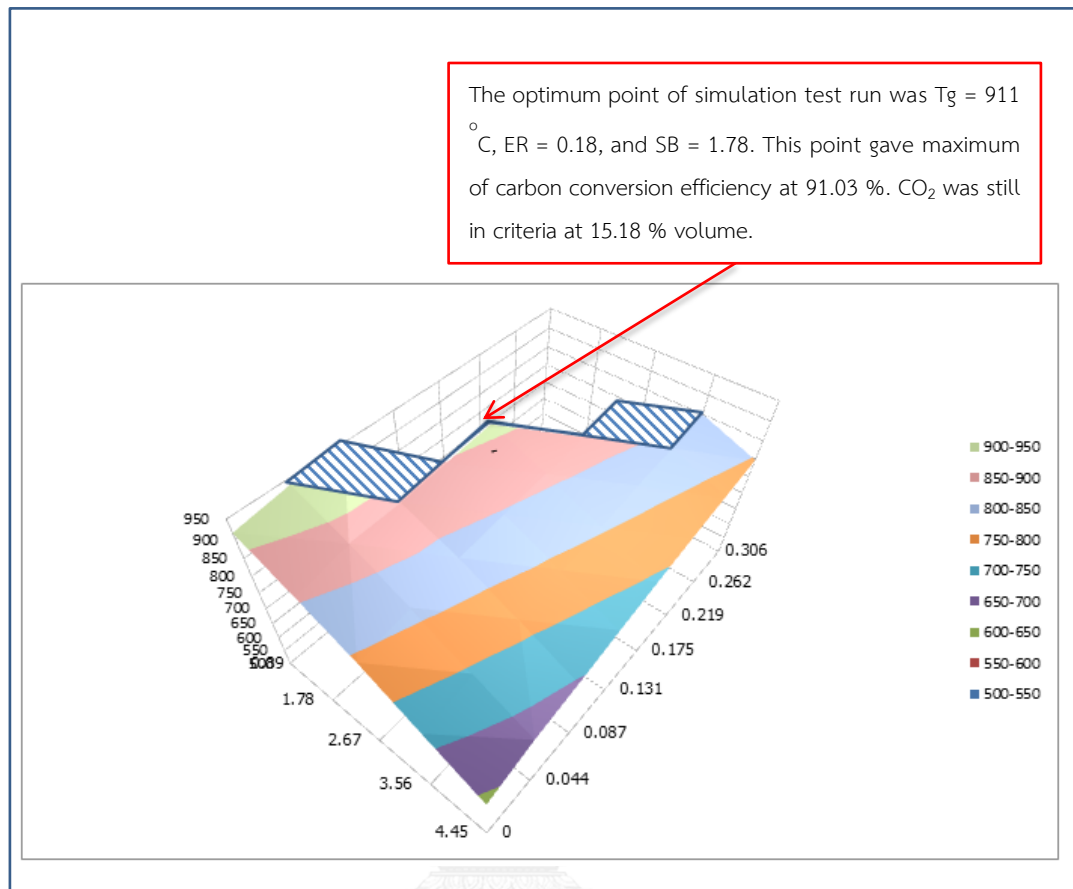


Fig. 33 The operating region for heat optimization result

Fig. 33 showed the shading region where the carbon conversion efficiency was higher than 70 percentages and carbon dioxide oxide gas was lower than 20 volumetric percentages. However, if no steam supplied, the energy self-sufficient condition cannot be found because there was no any endothermic energy produced by char gasification reaction to balance with the exothermic energy which occurred in pyrolysis and combustion zones. The optimized region could be only found when the steam-to-biomass ratio was between 0.89 and 3.56. If the steam-to-biomass ratio was above 3.56, the large amount of steam would be fed to the RCSTR reactor. This stream resulted in the reduction of carbon conversion ratio and it could not be achieved to 70 percent in any operating conditions.

CHAPTER VII

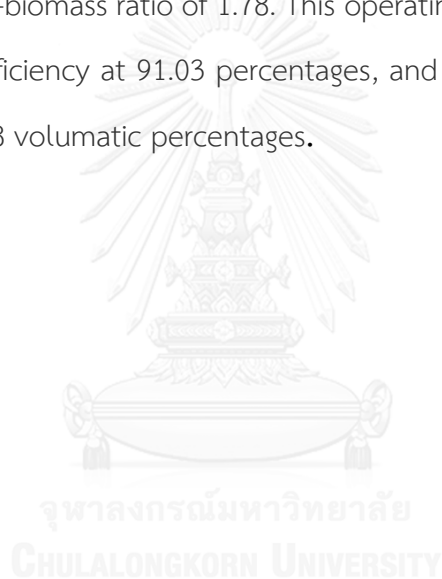
CONCLUSION

In this study, the thermodynamic equilibrium analysis of steam gasification process from biomass was done by substitution of gasification reactor with three sequencing reactors (RYIELD reactor, RGIBBS reactor, and RCSTR reactor) and using ASPEN PLUS simulator software. The biomass used for model validation was pine sawdust. The biomass gasification technology in this study was fluidized bed technology (conventional gasification). The effect of three operating parameters (gasification temperature, equivalence ratio, and steam-to-biomass ratio) were analyzed and compared with the experimental data. Then, the various types of Thai biomass such as rice husk, rice straw, maize stalk, and sugar cane were used for the simulation model in order to study the effect of gasification temperature on gas production composition and carbon conversion efficiency. However, the energy optimization of steam gasification process was the ultimate target of this study. The energy self-sufficient condition was that any energy was supplied to or removed from the gasification reactor. The energy self-sufficient condition could be achieved when gasification temperature, equivalence ratio, and steam-to-biomass ratio were properly selected.

The several unit operation blocks, including separation processes and many types of reactors in process simulation model by ASPEN PLUS gave good agreement with the experimental data. The simulation results showed that rise in temperature and steam-to-biomass ratio could improve the steam gasification process. Hydrogen and carbon conversion efficiency were increased but carbon dioxide, carbon monoxide, and methane were decreased with increasing of temperature and steam-to-biomass ratio. The increasing of equivalence ratio increased carbon dioxide, carbon

monoxide, and carbon conversion efficiency but the complete combustion had to be avoided in order to limit volumetric percentage of carbon dioxide in product gas.

Forty-eight batches of simulation test run were executed in order to find the relationship among gasification temperature, equivalence ratio, and steam-to-biomass ratio to obtain the energy self-sufficient condition. An equivalence ratio was varied from 0 to 0.31, and steam-to-biomass ratio was varied from 0 to 4.49. The gasification temperature was selected in range of 600 – 1000 °C. Finally, the optimum point of simulation test run was found at gasification temperature of 911 °C, equivalence ratio of 0.18, and steam-to-biomass ratio of 1.78. This operating point gave the maximum of carbon conversion efficiency at 91.03 percentages, and carbon dioxide oxide gas was still in criteria at 15.18 volumatic percentages.



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APPENDIX

จุฬาลงกรณ์มหาวิทยาลัย
CHULALONGKORN UNIVERSITY

THE EXAMPLE CALCULATION OF EQUIVALENCE RATIO (ER)

Refer to Fig. 15, biomass was fed at flow rate 0.512 kg/h. The flow rate of air supply was varied in range of 0.5 – 0.7 Nm³/h. The calculation of equivalence ratio can be performed as follows.

Air supply at 0.5 Nm³/h

$$\begin{aligned} \text{Weight of oxygen (air)} &= (\text{Flowrate of air}) \times (\text{density of air}) \times (\text{O}_2 \text{ wt.\% of air}) \\ &= (0.5 \text{ Nm}^3/\text{h}) \times (1.225 \text{ kg/Nm}^3) \times (0.23) = 0.141 \text{ kg/h} \end{aligned}$$

$$\begin{aligned} \text{Weight of dry biomass} &= (\text{Flow rate of biomass}) \times (1 - \text{moisture wt.\%}) \\ &= (0.512 \text{ kg/h}) \times (1 - 0.08) = 0.471 \text{ kg/h} \end{aligned}$$

$$\text{Stoichiometric ratio of oxygen (air)/biomass} = 1.44$$

$$\text{ER} = \frac{\text{weight of oxygen (air)/weight of dry biomass}}{\text{stoichiometric of oxygen (air)/biomass}}$$

$$\text{ER} = \frac{(0.129 \text{ kg/h})/(0.471 \text{ kg/h})}{1.44} = 0.19$$

Table A1 The calculation of equivalence ratio

Air flow rate (Nm ³ /h)	Weight of oxygen (kg/h)	Weight of dry biomass (kg/h)	Stoichiometric ratio of oxygen (air)/biomass	Equivalence ratio (ER)
0.50	0.141	0.471	1.44	0.21
0.55	0.154	0.471	1.44	0.23
0.60	0.169	0.471	1.44	0.25
0.65	0.182	0.471	1.44	0.27
0.70	0.197	0.471	1.44	0.29

THE EXAMPLE CALCULATION OF STEAM-TO-BIOMASS RATIO (SB)

Refer to Fig. 20, biomass was fed at flow rate 0.445 kg/h. The flow rate of steam supply was varied in range of 0 – 1.8 kg/h. The calculation of steam-to-biomass ratio can be performed as follows.

Steam supply at 1.8 kg/h

$$\begin{aligned} \text{Weight of dry biomass} &= (\text{Flow rate of biomass}) \times (1 - \text{moisture wt.}\%) \\ &= (0.445 \text{ kg/h}) \times (1 - 0.08) = 0.409 \text{ kg/h} \end{aligned}$$

$$SB = \frac{\text{weight of steam}}{\text{weight of dry biomass}}$$

$$SB = \frac{(1.8 \text{ kg/h})}{(0.409 \text{ kg/h})} = 4.4$$

Table A2 The calculation of equivalence ratio

Steam flow rate (kg/h)	Weight of dry biomass (kg/h)	Equivalence ratio (ER)
0	0.409	0
0.6	0.409	1.5
0.9	0.409	2.2
1.2	0.409	2.9
1.8	0.409	4.4

SIMULATION DATA

Table A3 Input parameters for simulation model

Operation block	Operating condition	Information
<p style="text-align: center;">Reactor “DECOMP” (RYIELD)</p>	<p>Pressure: 1 atm Temperature: 400 °C</p>	<p>Input stream:</p> <ul style="list-style-type: none"> - Identify Non-conventional component of biomass <p>Output stream:</p> <ul style="list-style-type: none"> - Identify conventional components of C, H₂O, H₂, O₂, N₂, and S - Identify Non-conventional component of ash <p>Equations:</p> <ul style="list-style-type: none"> - H₂O = WATER / 100 - ASH = [ULT (1) / 100] × [(100 – WATER) / 100] - CARB = [ULT (2) / 100] × [(100 – WATER) / 100] - H₂ = [ULT (3) / 100] × [(100 – WATER) / 100] - N₂ = [ULT (4) / 100] × [(100 – WATER) / 100] - CL₂ = [ULT (5)/100] × [(100 – WATER) / 100] - SULF = [ULT (6)/100] × [(100 – WATER) / 100] - O₂ = [ULT (7)/100] × [(100 – WATER) / 100]
<p style="text-align: center;">Separation Column “CHAR-SEP”</p>	<p>Pressure: 1 atm Temperature: 400 °C</p>	<p>Input stream:</p> <ul style="list-style-type: none"> - N/A <p>Output stream:</p> <ul style="list-style-type: none"> - Separate C (solid) and ash to stream “CHAR” <p>Equations:</p> <ul style="list-style-type: none"> - CHAR = CARB – (FC / 100) × [(100 – WATER) / 100]

Table A3 Input parameters for simulation model (Continued)

Operation block	Operating condition	Information
<p style="text-align: center;">Reactor “VOLATILE” (RGIBBS)</p>	<p>Pressure: 1 atm Temperature: 500 °C</p>	<p>Input stream:</p> <ul style="list-style-type: none"> - N/A <p>Output stream:</p> <ul style="list-style-type: none"> - Identify conventional components of H₂O, H₂, O₂, N₂, Sulfur, CO, and CH₄ <p>Equations:</p> <ul style="list-style-type: none"> - $\Delta G_i^{\circ} = -RT \ln(K)$ - $G_i = \Delta G_i^{\circ} + RT \ln(P_i)$ - $\Delta G = \left(\sum_i^n G_i \right)_{\text{Product}} + \left(\sum_i^n G_i \right)_{\text{Reactant}}$
<p style="text-align: center;">Mixing Tank “MIXER”</p>	<p>Pressure: 1 atm Heat duty: 0</p>	<p>Input stream:</p> <ul style="list-style-type: none"> - Identify air feed stream - Identify steam feed stream <p>Output stream:</p> <ul style="list-style-type: none"> - N/A <p>Equations:</p> <ul style="list-style-type: none"> - N/A

Table A3 Input parameters for simulation model (Continued)

Operation block	Operating condition	Information
<p>Reactor "COM-RE" (RCSTR)</p>	<p>Pressure: 1 atm Temp.: 700 – 900 °C</p>	<p>Input stream: - N/A</p> <p>Output stream: - N/A</p> <p>Equations: - $C + 0.7O_2 \rightarrow 0.6CO + 0.4CO_2$ - $\frac{dX_{CO}}{dt} = k_{CO} \exp\left(\frac{-E_{CO}}{RT_g}\right) P_{O_2}^n (1 - X_{CO})^{\frac{2}{3}}$ - $k_{CO} = 0.046 \text{ s}^{-1} \text{ atm}^{-1}$, $E_{CO} = 1,166 \text{ K}$ - $C + 1.3H_2O \rightarrow 0.3CO_2 + 0.7CO + 1.3H_2$ - $\frac{dX_{SG}}{dt} = k_{SG} \exp\left(\frac{-E_{SG}}{RT_g}\right) P_{H_2O}^n (1 - X_{SG})^{\frac{2}{3}}$ - $K_{SG} = 6,474.7 \text{ s}^{-1} \text{ atm}^{-1}$, $E_{SG} = 19,544 \text{ K}$ - $r_C = \left(\frac{dX_{CO}}{dt} + \frac{dX_{SG}}{dt}\right) \times \frac{\rho_C \varepsilon_S Y_C}{M_C}$</p>
<p>Solid Removal "CYCLONE"</p>	<p>Pressure: 1 atm Heat duty: 0</p>	<p>Input stream: - N/A</p> <p>Output stream: - Separate solid components to stream "P-Solid"</p> <p>Equations: - N/A</p>

Table A4 The simulation result of gasification temperature effect

(biomass: 0.445 kg/h, air: 0.5 Nm³/h, steam: 1.2 kg/h)

Temp (°C)	ER	SB	Gas composition (% volume)				Carbon conversion (%)
			H ₂	CO	CO ₂	CH ₄	
700	0.22	2.67	30.20	40.68	19.41	9.71	71.98
750	0.22	2.67	31.73	40.23	19.11	8.92	73.43
800	0.22	2.67	36.11	38.45	18.05	7.39	76.81
850	0.22	2.67	41.61	36.19	16.69	5.51	83.57
900	0.22	2.67	45.98	34.55	15.64	3.83	95.65

Table A5 The simulation result of equivalence ratio effect

(biomass: 0.512 kg/h, temperature: 800 °C, steam: 0.8 kg/h)

ER	Temp (°C)	SB	Gas composition (% volume)				Carbon conversion (%)
			H ₂	CO	CO ₂	CH ₄	
0.19	800	1.56	35.62	38.62	17.66	8.10	70.42
0.21	800	1.56	34.44	39.36	18.36	7.83	72.94
0.23	800	1.56	33.42	39.93	19.06	7.60	75.46
0.25	800	1.56	32.38	40.58	19.67	7.36	77.98
0.27	800	1.56	31.48	41.08	20.29	7.15	80.50

Table A6 The simulation result of steam-to-biomass ratio effect

(biomass: 0.445 kg/h, air: 0.5 Nm³/h, steam: 1.2 kg/h)

SB	Temp (°C)	ER	Gas composition (% volume)				Carbon conversion (%)
			H ₂	CO	CO ₂	CH ₄	
0	800	0.22	31.07	40.78	19.42	8.74	71.69
1.35	800	0.22	34.38	39.29	18.60	7.74	75.07
2.02	800	0.22	36.25	38.37	17.97	7.41	76.04
2.67	800	0.22	36.11	38.45	18.05	7.39	76.52
4.04	800	0.22	35.97	38.54	18.13	7.36	77.00



Table A7 The simulation result of gasification temperature effect for various biomass types (biomass: 0.445 kg/h, air: 0.5 Nm³/h, steam: 1.2 kg/h)

Biomass type	Temp (°C)	ER	SB	Gas composition (% volume)				Carbon conversion (%)
				H ₂	CO	CO ₂	CH ₄	
Rice husk	700	0.22	2.67	13.34	70.98	14.85	0.83	72.95
	750	0.22	2.67	12.87	70.81	15.51	0.80	74.40
	800	0.22	2.67	21.46	63.23	14.63	0.67	77.78
	850	0.22	2.67	29.30	55.91	14.27	0.52	84.06
	900	0.22	2.67	36.52	49.13	13.97	0.38	95.65
Rice straw	700	0.22	2.67	30.99	42.06	17.26	9.69	43.48
	750	0.22	2.67	34.61	40.05	16.68	8.65	45.41
	800	0.22	2.67	36.26	39.71	16.48	7.55	48.31
	850	0.22	2.67	41.28	37.35	15.64	5.73	55.07
	900	0.22	2.67	45.61	35.37	14.96	4.07	66.18
Maize stalk	700	0.22	2.67	27.80	50.64	15.48	6.08	43.48
	750	0.22	2.67	31.25	48.22	15.06	5.47	45.41
	800	0.22	2.67	33.15	46.96	15.07	4.83	48.31
	850	0.22	2.67	38.53	43.12	14.60	3.75	55.07
	900	0.22	2.67	43.25	39.72	14.32	2.70	66.67
Sugar cane	700	0.22	2.67	28.73	47.20	16.00	8.08	40.58
	750	0.22	2.67	32.19	45.06	15.51	7.24	42.51
	800	0.22	2.67	34.02	44.14	15.46	6.38	45.41
	850	0.22	2.67	39.32	40.88	14.89	4.91	52.17
	900	0.22	2.67	45.59	36.90	14.09	3.42	63.77

Table A8 The simulation result for heat optimization of steam gasification process

Batch	ER	SB	Temp (°C)	Required energy (kJ/h)	Gas composition (% volume)				Carbon conversion (%)
					H ₂	CO	CO ₂	CH ₄	
#1	0	0	700	-1958	56.63	23.69	1.47	18.20	15.46
	0	0	750	-1850	56.50	24.72	2.89	15.89	17.87
	0	0	800	-1690	56.17	26.08	5.11	12.64	22.71
	0	0	850	-1470	55.48	27.74	7.18	9.60	29.95
	0	0	900	-1208	56.75	27.70	8.46	7.09	39.61
No energy self-sufficient condition with any gasification temperature									
#2	0.04	0	700	-2187	43.29	31.95	8.53	16.23	22.71
	0.04	0	750	-2084	44.57	31.84	9.26	14.33	25.12
	0.04	0	800	-1923	47.09	31.39	9.75	11.77	28.99
	0.04	0	850	-1715	46.48	32.65	12.15	8.72	40.10
	0.04	0	900	-1462	51.76	30.45	10.93	6.85	45.89
No energy self-sufficient condition with any gasification temperature									
#3	0.09	0	700	-2333	38.32	35.12	12.19	14.37	28.02
	0.09	0	750	-2239	40.53	34.33	12.11	13.03	29.95
	0.09	0	800	-2076	42.71	33.89	12.73	10.68	34.78
	0.09	0	850	-1865	46.07	32.91	12.39	8.64	40.58
	0.09	0	900	-1603	48.34	32.37	12.50	6.80	49.76
No energy self-sufficient condition with any gasification temperature									
#4	0.13	0	700	-2503	33.69	38.10	15.57	12.63	34.30
	0.13	0	750	-2409	35.83	37.29	15.36	11.52	36.23
	0.13	0	800	-2246	38.68	36.22	15.43	9.67	41.06
	0.13	0	850	-2035	43.02	34.57	14.34	8.07	45.89
	0.13	0	900	-1773	45.79	33.73	14.05	6.44	55.07
No energy self-sufficient condition with any gasification temperature									

Table A8 The simulation result for heat optimization of steam gasification process

(Continued)

Batch	ER	SB	Temp (°C)	Required energy (kJ/h)	Gas composition (% volume)				Carbon conversion (%)
					H ₂	CO	CO ₂	CH ₄	
#5	0.18	0	700	-2681	30.06	40.44	18.22	11.27	40.58
	0.18	0	750	-2571	32.46	39.41	17.70	10.43	42.03
	0.18	0	800	-2421	36.41	37.57	16.92	9.10	45.41
	0.18	0	850	-2214	38.12	37.38	16.70	7.80	51.69
	0.18	0	900	-1954	40.98	36.49	16.39	6.15	62.80
No energy self-sufficient condition with any gasification temperature									
#6	0.22	0	700	-2857	27.14	42.33	20.36	10.18	46.86
	0.22	0	750	-2745	29.51	41.26	19.74	9.49	48.31
	0.22	0	800	-2595	31.07	40.78	19.42	8.74	51.69
	0.22	0	850	-2390	35.70	38.71	18.29	7.30	57.49
	0.22	0	900	-2129	39.81	36.97	17.25	5.97	65.70
No energy self-sufficient condition with any gasification temperature									
#7	0.26	0	700	-3030	24.74	43.88	22.11	9.28	53.14
	0.26	0	750	-2917	27.14	42.64	21.50	8.72	54.59
	0.26	0	800	-2767	28.67	42.24	21.02	8.06	57.49
	0.26	0	850	-2563	33.56	39.88	19.69	6.86	63.29
	0.26	0	900	-2302	36.27	39.05	18.84	5.83	71.50
No energy self-sufficient condition with any gasification temperature									
#8	0.31	0	700	-3202	22.72	45.17	23.58	8.52	58.94
	0.31	0	750	-3087	25.05	43.96	22.93	8.05	60.87
	0.31	0	800	-2936	26.69	43.37	22.44	7.51	63.77
	0.31	0	850	-2733	29.58	42.25	21.51	6.66	69.08
	0.31	0	900	-2472	34.52	39.98	19.95	5.55	76.81
No energy self-sufficient condition with any gasification temperature									

Table A8 The simulation result for heat optimization of steam gasification process
(Continued)

Batch	ER	SB	Temp (°C)	Required energy (kJ/h)	Gas composition (% volume)				Carbon conversion (%)
					H ₂	CO	CO ₂	CH ₄	
#9	0	0.89	750	-1321	55.31	25.68	3.46	15.56	18.84
	0	0.89	800	-1079	55.79	26.81	5.99	11.41	25.12
	0	0.89	850	-722	55.55	28.27	8.36	7.81	37.20
	0	0.89	900	-225	56.55	28.60	9.77	5.09	55.56
	0	0.89	950	383	56.70	29.02	10.74	3.54	79.71
	0	0.89	916	0	56.34	28.89	10.24	4.53	62.80
#10	0.04	0.89	750	-1499	48.15	30.10	8.21	13.54	24.64
	0.04	0.89	800	-1263	50.74	29.65	9.23	10.38	30.92
	0.04	0.89	850	-920	51.23	30.65	10.92	7.20	43.96
	0.04	0.89	900	-441	53.21	30.41	11.39	4.99	60.87
	0.04	0.89	950	172	54.56	30.17	11.76	3.51	84.54
	0.04	0.89	936	0	53.82	30.51	11.76	3.91	76.81
#11	0.09	0.89	750	-1679	42.80	33.25	11.92	12.04	30.92
	0.09	0.89	800	-1443	42.93	34.34	13.07	9.66	38.65
	0.09	0.89	850	-1100	49.66	31.45	11.44	7.45	43.96
	0.09	0.89	900	-621	50.52	31.85	12.68	4.94	65.22
	0.09	0.89	969	241	52.83	31.28	12.76	3.13	98.07
	0.09	0.89	949	0	51.36	31.91	13.23	3.50	90.34
#12	0.13	0.89	750	-1854	38.39	35.99	14.83	10.80	37.20
	0.13	0.89	800	-1618	40.34	35.73	14.85	9.08	42.51
	0.13	0.89	850	-1275	45.00	34.07	14.18	6.75	53.14
	0.13	0.89	900	-796	48.68	32.80	13.76	4.76	70.05
	0.13	0.89	959	-77	50.90	32.20	13.62	3.27	97.58
	No energy self-sufficient condition with any gasification temperature								

Table A8 The simulation result for heat optimization of steam gasification process
(Continued)

Batch	ER	SB	Temp (°C)	Required energy (kJ/h)	Gas composition (% volume)				Carbon conversion (%)
					H ₂	CO	CO ₂	CH ₄	
#13	0.18	0.89	750	-2027	34.80	38.21	17.20	9.79	43.48
	0.18	0.89	800	-1792	37.28	37.55	16.78	8.39	48.79
	0.18	0.89	850	-1453	42.50	35.42	15.71	6.37	58.94
	0.18	0.89	900	-985	44.94	34.87	15.60	4.60	78.26
	0.18	0.89	949	-392	48.74	33.29	14.54	3.43	97.58
No energy self-sufficient condition with any gasification temperature									
#14	0.22	0.89	750	-2199	31.97	39.96	19.07	8.99	49.28
	0.22	0.89	800	-1964	34.66	39.11	18.43	7.80	54.59
	0.22	0.89	850	-1629	38.61	37.63	17.55	6.21	64.25
	0.22	0.89	900	-1159	43.08	35.90	16.41	4.62	80.68
	0.22	0.89	944	-638	46.54	34.46	15.51	3.49	99.52
No energy self-sufficient condition with any gasification temperature									
#15	0.26	0.89	750	-2368	26.75	43.12	21.54	8.60	55.56
	0.26	0.89	800	-2134	32.33	40.41	19.99	7.27	60.39
	0.26	0.89	850	-1801	36.68	38.73	18.70	5.89	70.05
	0.26	0.89	900	-1336	41.51	36.71	17.34	4.45	85.99
	0.26	0.89	933	-955	43.97	35.71	16.66	3.66	99.52
No energy self-sufficient condition with any gasification temperature									
#16	0.31	0.89	750	-2536	24.72	44.39	22.95	7.94	61.84
	0.31	0.89	800	-2302	30.34	41.60	21.24	6.83	66.67
	0.31	0.89	850	-1972	34.88	39.69	19.82	5.61	75.85
	0.31	0.89	900	-1510	40.05	37.46	18.20	4.29	91.30
	0.31	0.89	922	-1263	42.02	36.62	17.57	3.78	99.52
No energy self-sufficient condition with any gasification temperature									

Table A8 The simulation result for heat optimization of steam gasification process
(Continued)

Batch	ER	SB	Temp (°C)	Required energy (kJ/h)	Gas composition (% volume)				Carbon conversion (%)
					H ₂	CO	CO ₂	CH ₄	
#17	0	1.78	700	-1023	56.31	24.13	1.46	18.10	15.94
	0	1.78	750	-806	54.87	25.96	3.74	15.43	18.84
	0	1.78	800	-507	55.13	27.21	6.38	11.28	26.09
	0	1.78	850	-69	55.55	28.48	8.62	7.35	39.61
	0	1.78	900	560	56.69	28.63	10.12	4.56	61.84
	0	1.78	856	0	55.68	28.50	8.86	6.96	41.55
#18	0.04	1.78	700	-1202	47.86	29.30	7.46	15.38	22.22
	0.04	1.78	750	-984	47.82	30.31	8.42	13.45	25.12
	0.04	1.78	800	-685	50.04	30.22	9.51	10.23	31.88
	0.04	1.78	850	-246	51.04	30.88	11.33	6.76	47.34
	0.04	1.78	900	371	53.87	30.21	11.43	4.49	67.15
	0.04	1.78	880	0	52.68	30.61	11.32	5.39	57.49
#19	0.09	1.78	700	-1379	41.73	33.21	11.65	13.41	28.50
	0.09	1.78	750	-1158	42.53	33.42	12.08	11.96	31.40
	0.09	1.78	800	-871	45.49	32.79	12.41	9.31	38.16
	0.09	1.78	850	-420	48.26	32.45	12.90	6.39	52.66
	0.09	1.78	900	196	48.91	32.92	13.94	4.23	78.74
	0.09	1.78	884	0	48.92	32.66	13.63	4.79	69.57
#20	0.13	1.78	700	-1553	36.99	36.23	14.89	11.89	34.78
	0.13	1.78	750	-1331	38.17	36.13	14.97	10.74	37.68
	0.13	1.78	800	-1033	42.04	34.94	14.42	8.60	43.96
	0.13	1.78	850	-590	42.65	35.60	15.75	6.00	62.32
	0.13	1.78	900	28	49.41	32.58	13.73	4.28	77.29
	0.13	1.78	898	0	48.72	32.99	13.91	4.38	76.33

Table A8 The simulation result for heat optimization of steam gasification process
(Continued)

Batch	ER	SB	Temp (°C)	Required energy (kJ/h)	Gas composition (% volume)				Carbon conversion (%)
					H ₂	CO	CO ₂	CH ₄	
#21	0.18	1.78	700	-1724	33.22	38.64	17.47	10.68	40.58
	0.18	1.78	750	-1501	34.69	38.41	17.15	9.76	43.48
	0.18	1.78	800	-1204	39.01	36.73	16.28	7.98	49.76
	0.18	1.78	850	-780	42.86	35.40	15.71	6.03	61.84
	0.18	1.78	900	-147	49.74	32.40	13.38	4.48	73.43
	0.18	1.78	911	0	46.99	34.05	15.18	3.78	91.30
#22	0.22	1.78	750	-1670	31.73	40.23	19.11	8.92	49.76
	0.22	1.78	800	-1373	34.16	39.53	18.63	7.69	55.56
	0.22	1.78	850	-952	40.77	36.58	16.91	5.73	67.63
	0.22	1.78	900	-353	45.30	34.81	15.81	4.08	87.44
	0.22	1.78	922	-24	47.54	34.39	15.53	3.49	99.52
No energy self-sufficient condition with any gasification temperature									
#23	0.26	1.78	750	-1836	29.36	41.69	20.69	8.26	56.04
	0.26	1.78	800	-1540	31.94	40.84	20.04	7.19	61.84
	0.26	1.78	850	-1122	37.24	38.66	18.51	5.59	72.95
	0.26	1.78	900	-527	42.83	36.20	16.95	4.02	92.75
	0.26	1.78	913	-339	44.00	35.74	16.59	3.67	99.52
No energy self-sufficient condition with any gasification temperature									
#24	0.31	1.78	750	-2001	27.28	42.87	22.17	7.67	61.84
	0.31	1.78	800	-1705	29.99	41.99	21.27	6.75	67.63
	0.31	1.78	850	-1289	35.51	39.57	19.59	5.33	78.74
	0.31	1.78	900	-699	41.47	36.90	17.75	3.89	98.07
	0.31	1.78	903	-657	41.11	37.20	17.83	3.85	99.52
No energy self-sufficient condition with any gasification temperature									

Table A8 The simulation result for heat optimization of steam gasification process
(Continued)

Batch	ER	SB	Temp (°C)	Required energy (kJ/h)	Gas composition (% volume)				Carbon conversion (%)
					H ₂	CO	CO ₂	CH ₄	
#25	0	2.67	700	-559	56.10	24.04	1.82	18.03	15.94
	0	2.67	750	-295	54.87	25.96	3.74	15.43	18.84
	0	2.67	800	57	56.77	26.36	6.24	10.64	26.09
	0	2.67	850	560	56.21	28.11	8.66	7.03	40.58
	0	2.67	900	1285	56.19	29.06	10.39	4.36	65.70
	0	2.67	793	0	56.12	26.60	5.80	11.48	25.12
#26	0.04	2.67	700	-737	47.86	29.30	7.46	15.38	22.22
	0.04	2.67	750	-470	47.82	30.31	8.42	13.45	25.12
	0.04	2.67	800	-118	49.61	30.60	9.64	10.15	32.37
	0.04	2.67	850	382	52.97	29.85	10.57	6.62	46.38
	0.04	2.67	900	1101	54.29	30.09	11.40	4.21	70.53
	0.04	2.67	814	0	51.58	29.76	9.74	8.93	35.27
#27	0.09	2.67	700	-911	41.73	33.21	11.65	13.41	28.50
	0.09	2.67	750	-643	42.37	33.67	12.04	11.92	31.40
	0.09	2.67	800	-291	45.36	32.99	12.37	9.28	38.16
	0.09	2.67	850	207	48.65	32.30	12.62	6.44	52.17
	0.09	2.67	900	920	51.67	31.51	12.67	4.15	75.85
	0.09	2.67	832	0	48.58	31.92	12.22	7.29	45.89
#28	0.13	2.67	700	-1082	36.99	36.23	14.89	11.89	34.30
	0.13	2.67	750	-814	38.04	36.34	14.91	10.70	37.68
	0.13	2.67	800	-462	40.24	36.06	15.47	8.23	47.34
	0.13	2.67	850	36	43.45	35.23	15.57	5.75	64.25
	0.13	2.67	900	749	49.97	32.38	13.63	4.02	81.16
	0.13	2.67	847	0	43.92	34.88	15.38	5.81	62.80

Table A8 The simulation result for heat optimization of steam gasification process
(Continued)

Batch	ER	SB	Temp (°C)	Required energy (kJ/h)	Gas composition (% volume)				Carbon conversion (%)
					H ₂	CO	CO ₂	CH ₄	
#29	0.18	2.67	700	-1251	33.29	38.72	17.29	10.70	40.58
	0.18	2.67	750	-980	34.69	38.41	17.15	9.76	43.96
	0.18	2.67	800	-628	38.69	36.93	16.47	7.91	50.24
	0.18	2.67	850	-136	43.71	35.08	15.43	5.79	63.29
	0.18	2.67	900	567	47.47	33.78	14.79	3.96	86.47
	0.18	2.67	861	0	44.87	34.58	15.24	5.31	67.63
#30	0.22	2.67	700	-1417	30.20	40.68	19.41	9.71	46.86
	0.22	2.67	750	-1146	31.73	40.23	19.11	8.92	49.76
	0.22	2.67	800	-794	36.11	38.45	18.05	7.39	56.52
	0.22	2.67	850	-304	41.61	36.19	16.69	5.51	69.08
	0.22	2.67	900	394	45.98	34.55	15.64	3.83	91.79
	0.22	2.67	873	0	43.73	35.40	16.19	4.69	78.26
#31	0.26	2.67	700	-1581	27.77	42.22	21.09	8.92	52.66
	0.26	2.67	750	-1310	29.36	41.69	20.69	8.26	56.04
	0.26	2.67	800	-958	33.85	39.78	19.44	6.92	62.32
	0.26	2.67	850	-471	38.26	38.09	18.26	5.38	74.88
	0.26	2.67	900	223	43.65	35.86	16.71	3.78	97.10
	0.26	2.67	832	0	42.74	36.10	16.98	4.18	89.37
#32	0.31	2.67	700	-1743	25.69	43.52	22.52	8.26	58.45
	0.31	2.67	750	-1471	27.22	43.01	22.11	7.65	61.84
	0.31	2.67	800	-1120	31.86	40.96	20.67	6.52	68.12
	0.31	2.67	850	-635	36.49	39.10	19.28	5.13	80.68
	0.31	2.67	895	-26	42.11	36.57	17.53	3.79	99.99
	No energy self-sufficient condition with any gasification temperature								

Table A8 The simulation result for heat optimization of steam gasification process

(Continued)

Batch	ER	SB	Temp (°C)	Required energy (kJ/h)	Gas composition (% volume)				Carbon conversion (%)
					H ₂	CO	CO ₂	CH ₄	
#33	0	3.56	700	-94	56.10	24.04	1.82	18.03	15.94
	0	3.56	750	217	54.87	25.96	3.74	15.43	19.32
	0	3.56	800	619	56.77	26.36	6.24	10.64	26.57
	0	3.56	850	1180	55.68	28.50	8.86	6.96	41.55
	0	3.56	900	1984	56.17	29.15	10.47	4.21	67.63
	0	3.56	716	0	54.96	25.24	2.14	17.67	16.43
#34	0.04	3.56	700	-272	47.86	29.30	7.46	15.38	22.22
	0.04	3.56	750	42	47.82	30.31	8.42	13.45	25.60
	0.04	3.56	800	444	49.35	30.76	9.79	10.09	32.85
	0.04	3.56	850	1004	52.50	30.21	10.74	6.56	47.34
	0.04	3.56	900	1676	53.24	30.67	12.10	3.99	76.33
	0.04	3.56	744	0	48.15	30.10	8.21	13.54	24.64
#35	0.09	3.56	700	-444	41.73	33.21	11.65	13.41	28.50
	0.09	3.56	750	-129	42.37	33.67	12.04	11.92	31.40
	0.09	3.56	800	274	45.23	33.19	12.33	9.25	38.65
	0.09	3.56	850	778	48.93	32.23	12.73	6.12	54.59
	0.09	3.56	900	1626	51.69	31.58	12.72	4.01	78.26
	0.09	3.56	767	0	43.77	33.35	11.94	10.94	33.33
#36	0.13	3.56	700	-613	37.08	36.32	14.69	11.92	34.30
	0.13	3.56	750	-296	38.04	36.34	14.91	10.70	37.68
	0.13	3.56	800	108	45.23	33.19	12.33	9.25	38.65
	0.13	3.56	850	663	46.59	33.46	14.12	5.82	59.42
	0.13	3.56	900	1357	50.05	32.42	13.65	3.88	84.06
	0.13	3.56	788	0	44.63	33.15	12.17	10.04	35.75

Table A8 The simulation result for heat optimization of steam gasification process

(Continued)

Batch	ER	SB	Temp (°C)	Required energy (kJ/h)	Gas composition (% volume)				Carbon conversion (%)
					H ₂	CO	CO ₂	CH ₄	
#37	0.18	3.56	700	-779	33.29	38.72	17.29	10.70	40.58
	0.18	3.56	750	-462	34.58	38.60	17.09	9.73	43.96
	0.18	3.56	800	-58	38.59	37.09	16.43	7.89	50.72
	0.18	3.56	850	495	43.24	35.43	15.61	5.72	64.73
	0.18	3.56	900	1187	46.94	34.13	15.16	3.77	91.79
	0.18	3.56	806	0	40.20	36.13	16.14	7.54	51.69
#38	0.22	3.56	700	-943	30.35	40.57	19.32	9.76	46.38
	0.22	3.56	750	-625	31.73	40.23	19.11	8.92	49.76
	0.22	3.56	800	-222	35.97	38.54	18.13	7.36	56.52
	0.22	3.56	850	330	41.19	36.51	16.85	5.45	70.05
	0.22	3.56	900	1110	46.18	34.52	15.59	3.71	94.69
	0.22	3.56	822	0	37.91	37.91	17.63	6.56	61.84
#39	0.26	3.56	700	-1103	27.89	42.13	21.01	8.97	52.66
	0.26	3.56	750	-785	29.36	41.69	20.69	8.26	55.56
	0.26	3.56	800	-383	33.73	39.86	19.51	6.90	62.80
	0.26	3.56	850	166	39.36	37.54	17.89	5.21	75.85
	0.26	3.56	900	943	44.82	35.21	16.37	3.60	99.52
	0.26	3.56	837	0	37.75	38.29	18.30	5.66	71.50
#40	0.31	3.56	700	-1261	25.80	43.45	22.45	8.29	58.45
	0.31	3.56	750	-944	27.33	42.94	22.05	7.69	61.84
	0.31	3.56	800	-542	31.75	41.03	20.73	6.49	68.60
	0.31	3.56	850	0	37.59	38.54	18.90	4.98	81.64

Table A8 The simulation result for heat optimization of steam gasification process

(Continued)

Batch	ER	SB	Temp (°C)	Required energy (kJ/h)	Gas composition (% volume)				Carbon conversion (%)
					H ₂	CO	CO ₂	CH ₄	
#41	0	4.45	550	-500	55.58	23.16	0.42	20.84	14.01
	0	4.45	600	-227	55.21	23.66	0.42	20.71	14.01
	0	4.45	650	59	54.27	24.55	0.82	20.35	14.49
	0	4.45	700	369	56.10	24.04	1.82	18.03	15.94
	0	4.45	640	0	54.85	24.16	0.42	20.57	14.49
#42	0.04	4.45	600	-408	46.26	29.74	6.66	17.35	20.29
	0.04	4.45	650	-119	45.44	30.29	7.23	17.04	20.77
	0.04	4.45	700	193	47.86	29.30	7.46	15.38	22.22
	0.04	4.45	750	553	47.61	30.61	8.39	13.39	25.60
	0.04	4.45	670	0	45.04	30.56	7.51	16.89	21.26
#43	0.09	4.45	650	-291	39.19	34.53	11.58	14.70	27.05
	0.09	4.45	700	23	41.73	33.21	11.65	13.41	28.50
	0.09	4.45	750	385	42.37	33.67	12.04	11.92	31.40
	0.09	4.45	800	837	45.01	33.32	12.46	9.21	39.13
	0.09	4.45	696	0	41.84	33.30	11.41	13.45	28.02
#44	0.13	4.45	650	-459	34.60	37.48	14.94	12.98	32.85
	0.13	4.45	700	-144	37.08	36.32	14.69	11.92	34.30
	0.13	4.45	750	219	38.04	36.34	14.91	10.70	37.68
	0.13	4.45	800	672	41.56	35.35	14.60	8.50	37.68
	0.13	4.45	721	0	36.27	37.01	15.07	11.66	35.27

Table A8 The simulation result for heat optimization of steam gasification process

(Continued)

Batch	ER	SB	Temp (°C)	Required energy (kJ/h)	Gas composition (% volume)				Carbon conversion (%)
					H ₂	CO	CO ₂	CH ₄	
#45	0.18	4.45	650	-623	30.97	39.82	17.60	11.61	38.65
	0.18	4.45	700	-308	33.47	38.60	17.17	10.76	40.58
	0.18	4.45	750	56	34.58	38.60	17.09	9.73	43.96
	0.18	4.45	800	509	38.43	37.19	16.52	7.86	50.72
	0.18	4.45	743	0	34.98	38.10	17.09	9.84	43.00
#46	0.22	4.45	700	-468	30.51	40.47	19.22	9.81	46.38
	0.22	4.45	750	-105	31.79	40.30	18.97	8.94	49.76
	0.22	4.45	800	348	35.89	38.68	18.09	7.34	57.00
	0.22	4.45	850	956	41.00	36.69	16.88	5.43	71.01
	0.22	4.45	763	0	33.79	39.16	18.60	8.45	51.21
#47	0.26	4.45	700	-626	28.03	42.04	20.93	9.01	52.17
	0.26	4.45	750	-263	29.41	41.76	20.56	8.27	55.56
	0.26	4.45	800	189	33.65	39.99	19.47	6.88	62.80
	0.26	4.45	850	796	39.08	37.77	17.97	5.17	76.81
	0.26	4.45	780	0	32.83	40.09	19.70	7.39	59.42
#48	0.31	4.45	700	-781	25.92	43.37	22.38	8.33	57.97
	0.31	4.45	750	-419	27.37	43.01	21.93	7.70	61.35
	0.31	4.45	800	32	31.68	41.15	20.69	6.48	68.60
	0.31	4.45	850	637	37.40	38.65	19.00	4.95	82.61
	0.31	4.45	797	0	31.90	41.01	20.56	6.52	68.12

VITA

Siripong Limprachaya was born on the 10th of April, 1986 in Bangkok. He attended Worasarn Pittaya and Wat Suthi Vararam School for primary and secondary education. By taking the science-mathematic program in high school, he were interested in the field of engineering. Started in 2004, he undertook Bachelor of Engineering course in Mechanical Engineering at Chulalongkorn University and eventually graduated in 2008. Since his graduation, Siripong has already worked in many functions. He started off as a machinery engineer in Toyo-Thai Public Company Limited, then moved to SCG-DOW Chemical Company Limited as a critical rotating equipment engineer of maintenance section. In an attempt to find more challenging task, he is now working as a maintenance engineer (mechanical) in PTT Exploration and Production Public Company Limited. To take the challenge further, he decided to undertake a Master's degree in Chemical Engineering at Chulalongkorn University, where he studied in the field of Computational Process Engineering. His graduation is expected to be around December 2015.