

การออกแบบกระบวนการของการผลิตไฮโดรเจนสีเขียวจากการแก๊สซิฟิเคชัน
ของขานอ้อยร่วมกับกระบวนการดูดซับด้วยแคลเซียมออกไซด์

PROCESS DESIGN OF GREEN HYDROGEN PRODUCTION VIA BAGASSE
GASIFICATION INTEGRATED WITH CALCIUM OXIDE ADSORPTION
PROCESS



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วิทยานิพนธ์นี้เป็นส่วนหนึ่งของการศึกษาตามหลักสูตรปริญญาวิศวกรรมศาสตรมหาบัณฑิต

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เอกสารนี้เป็นเอกสารที่สงวนไว้สำหรับการใช้งานเพื่อการศึกษาเท่านั้น ไม่อนุญาตให้นำไปใช้ประโยชน์ด้านการค้า
ไม่ว่ากรณีใดๆ ทั้งสิ้น อีกทั้งห้ามมิให้ดัดแปลงเนื้อหา และต้องอ้างอิงถึงเจ้าของเอกสารทุกครั้งที่มีการนำไปใช้

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Thesis	Process Design of Green Hydrogen Production via Bagasse Gasification Integrated with Calcium Oxide Adsorption Process
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ABSTRACT

This project focuses on the production of green hydrogen from bagasse gasification integrated with calcium oxide (CaO) adsorption. Green hydrogen refers to hydrogen produced from renewable energy sources such as wind, solar, hydropower, geothermal energy, or biomass, making it eco-friendly with minimal to zero greenhouse gas emissions. Aspen Plus version 12 simulation software was employed to design and simulate the green hydrogen process. Steam and supercritical water were used as gasifying agents in the biomass gasification process. To improve hydrogen production, the bagasse gasification was to be integrated with the water gas shift process. Furthermore, the CaO adsorption was subsequently implemented for CO₂ capture. Simulation results revealed that the steam gasification integrated with CaO adsorption (SG-CaO) should be conducted at a gasifier temperature of 950 °C, a gasifier pressure of 1 bar, a steam to biomass mass ratio of 0.1, a water gas shift reactor temperature of 150 °C, a water to biomass mass ratio of 0.6, a carbonator temperature of 750 °C, a CaO to biomass mass ratio of 1.9, and a regenerator temperature of 900 °C. This integration results in the production of green hydrogen with a purity of 99.95%. Supercritical water gasification integrated with CaO adsorption

เอกสารนี้เป็นเอกสารที่สงวนไว้สำหรับการใช้งานเพื่อการศึกษาเท่านั้น ไม่อนุญาตให้นำไปใช้ประโยชน์ด้านการค้า
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(SCWG-CaO) should be carried out at a gasifier temperature of 1200 °C, a gasifier pressure of 221 bar, a supercritical water to biomass mass ratio of 0.4, a water gas shift reactor temperature of 150 °C, a water to biomass mass ratio of 0.2, a carbonator temperature of 800 °C, a CaO to biomass mass ratio of 1.78, and a regenerator temperature of 900 °C. This integration leads to the production of green hydrogen with a purity of 99.98%. When an energy analysis of both processes was performed, it was found that the energy efficiency of SG-CaO (41.42%) is superior to that of SCWG-CaO (26.01%). From our study, it can be concluded that the steam gasification of bagasse integrated with CaO adsorption is suitable for green hydrogen production.

Keywords: Hydrogen, Bagasse, Gasification, CO₂ capture, Process simulation



หัวข้อวิทยานิพนธ์	การออกแบบกระบวนการของการผลิตไฮโดรเจนสีเขียวจากการ แก๊สซิฟิเคชันของชานอ้อยร่วมกับกระบวนการดูดซับด้วย แคลเซียมออกไซด์
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บทคัดย่อ

โครงการนี้มุ่งเน้นการผลิตไฮโดรเจนสีเขียวที่เป็นมิตรต่อสิ่งแวดล้อมจากกระบวนการแก๊สซิฟิเคชันของชานอ้อยร่วมกับการดูดซับคาร์บอนไดออกไซด์ด้วยตัวดูดซับแคลเซียมออกไซด์ ไฮโดรเจนสีเขียวหมายถึงไฮโดรเจนที่ผลิตขึ้นโดยใช้แหล่งพลังงานหมุนเวียน เช่น ลม แสงอาทิตย์ ไฟฟ้าพลังน้ำ พลังงานความร้อนใต้พิภพ หรือชีวมวล ทำให้เป็นมิตรกับสิ่งแวดล้อมโดยปล่อยก๊าซเรือนกระจกน้อยที่สุดถึงศูนย์ ซอฟต์แวร์สำเร็จรูป Aspen Plus เวอร์ชัน 12 ถูกใช้เพื่อออกแบบและจำลองกระบวนการไฮโดรเจนสีเขียว โดยที่ไอน้ำและน้ำเหนือวิกฤตจะถูกใช้เป็นสารที่ช่วยให้เกิดปฏิกิริยาในกระบวนการแก๊สซิฟิเคชันของชีวมวล เพื่อเพิ่มการผลิตไฮโดรเจน กระบวนการแก๊สซิฟิเคชันของชานอ้อยควรร่วมกับการบวนการปฏิกิริยาเปลี่ยนน้ำเป็นแก๊ส นอกจากนี้การดูดซับด้วยแคลเซียมออกไซด์จะถูกนำมาใช้สำหรับการดักจับคาร์บอนไดออกไซด์ ผลการจำลองบ่งชี้ว่ากระบวนการแก๊สซิฟิเคชันของไอน้ำร่วมกับการดูดซับคาร์บอนไดออกไซด์ด้วยตัวดูดซับแคลเซียมออกไซด์ควรดำเนินการที่อุณหภูมิเตาแก๊สซิฟายเออร์ 950 องศาเซลเซียส ความดันเตาแก๊สซิฟายเออร์ 1 บาร์ สัดส่วนโดยมวลของไอน้ำต่อชีวมวลเท่ากับ 0.1 อุณหภูมิเครื่องปฏิกรณ์เปลี่ยนน้ำเป็นแก๊ส 150 องศาเซลเซียส สัดส่วนโดยมวลของน้ำต่อชีวมวลเท่ากับ 0.6 อุณหภูมิของเครื่องคาร์บอนเตอรที่ 750 องศาเซลเซียส สัดส่วนโดยมวลแคลเซียมออกไซด์ต่อชีวมวลเท่ากับ 1.9 และอุณหภูมิของเครื่องรีเจนเนอเรเตอร์ที่ 900 องศาเซลเซียส โดยกระบวนการนี้ได้รับการผลิตไฮโดรเจนสีเขียวที่มีระดับความบริสุทธิ์ร้อยละ 99.95 สำหรับกระบวนการแก๊สซิฟิเคชันของน้ำเหนือวิกฤตของชานอ้อยที่ร่วมกับการดูดซับคาร์บอนไดออกไซด์ด้วยตัวดูดซับแคลเซียมออกไซด์ควรดำเนินการที่อุณหภูมิของเตาแก๊สซิฟายเออร์ 1200 องศาเซลเซียส

ความดันของเตาแก๊สซีฟายเออร์ที่ 221 บาร์ สกัดส่วนโดยมวลของน้ำเหนือวิกฤตต่อชีวมวลเท่ากับ 0.4 อุณหภูมิของเครื่องปฏิกรณ์เปลี่ยนน้ำเป็นแก๊ส 150 องศาเซลเซียส สกัดส่วนโดยมวลของน้ำต่อชีวมวลเท่ากับ 0.2 อุณหภูมิของเครื่องคาร์บอนเตอร 800 องศาเซลเซียส สกัดส่วนโดยมวลของแคลเซียมออกไซด์ต่อชีวมวลเท่ากับ 1.78 และอุณหภูมิของเครื่องรีเจนเนอเรเตอร์ 900 องศาเซลเซียส โดยกระบวนการนี้ได้รับการผลิตไฮโดรเจนสีเขียวที่มีระดับความบริสุทธิ์ร้อยละ 99.98 เมื่อพิจารณาประสิทธิภาพพลังงานพบว่ากระบวนการแก๊สซิฟิเคชันของไอน้ำร่วมกับการดูดซับคาร์บอนไดออกไซด์ด้วยตัวดูดซับแคลเซียมออกไซด์ (41.42 เปอร์เซ็นต์) มีประสิทธิภาพทางพลังงานสูงกว่ากระบวนการแก๊สซิฟิเคชันของน้ำเหนือวิกฤตของซานอ้อยที่ร่วมกับการดูดซับคาร์บอนไดออกไซด์ด้วยตัวดูดซับแคลเซียมออกไซด์ (26.01 เปอร์เซ็นต์) ดังนั้นจึงสรุปได้ว่ากระบวนการกระบวนการแก๊สซิฟิเคชันของไอน้ำร่วมกับการดูดซับคาร์บอนไดออกไซด์ด้วยตัวดูดซับแคลเซียมออกไซด์มีความเหมาะสมในการผลิตไฮโดรเจนสีเขียว

คำสำคัญ: ไฮโดรเจน, ซานอ้อย, แก๊สซิฟิเคชัน, การดักจับคาร์บอนไดออกไซด์, การจำลองกระบวนการ

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Nitsara Panichkittikul

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CHAPTER I

INTRODUCTION

1.1 Background

The issue of carbon emissions and the resulting greenhouse effect has become a major concern worldwide. The world is constantly looking for ways to reduce carbon emissions, and hydrogen production is providing to be one of the most promising solutions. Hydrogen is a versatile and clean fuel that has the potential to revolutionize the way we power our homes, vehicles, and industries. The benefits of hydrogen as a clean fuel are well known.

Hydrogen¹ is a clean and renewable fuel that can be used in fuel cells to generate electricity and heat. It can also be used as a fuel for vehicles, and as a feedstock for the chemical industry. Hydrogen is an efficient and environmentally friendly energy source in which the combustion process produces only water vapor and heat. It is also highly versatile, as it can be produced from a variety of feedstocks, including natural gas, coal, and biomass. This work focuses on green hydrogen which is hydrogen gas generated through renewable energy sources such as wind, solar, hydropower, geothermal energy, or biomass, rather than relying on fossil fuels. The term "green" highlights its eco-friendly production process, which results in minimal to zero greenhouse gas emissions.

Biomass², which includes organic materials such as agricultural and forestry waste, is a promising feedstock for hydrogen production because it is abundant, renewable, and found in many countries, including Thailand. Thailand is an agricultural country that generates a large amount of biomass waste such as bagasse, rice husks, and coconut shells. The use of biomass for hydrogen production not only reduces the amount of waste, but also increases the value of agricultural residues

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that would otherwise be discarded. Biomass can be converted to hydrogen through a process called gasification. Gasification involves heating biomass in the presence of a gasifying agent such as steam, oxygen, or supercritical water to produce a mixture of hydrogen, carbon monoxide, and carbon dioxide. The efficiency of gasification depends on various factors such as the quality of the feedstock, gasifying agent, and the operating conditions.

Motta et al.³ conducted a study focusing on optimizing sugarcane bagasse gasification conditions to produce syngas mixtures for potential use in the production of liquid fuels and chemicals. This research analyzed various parameters, including temperature, pressure, steam-to-biomass ratio, moisture content, fluidized bed configurations, and gasifying media, to understand their effects on syngas composition and process performance. Their study revealed that temperature played a critical role in increasing CO generation and decreasing CO₂ formation during sugarcane bagasse gasification. Among the assessed scenarios, the circulating fluidized bed reactor demonstrated the most suitable performance, leading to higher H₂ and CO generation, lower CO₂ and CH₄ production, as well as improved H₂/CO ratio, dry syngas flow rates, and cold gas efficiency. The use of oxygen as an oxidizing agent, however, reduced H₂ content and increased CO concentration, resulting in a lower syngas H₂/CO ratio, lower heating value, and reduced cold gas efficiency. The study recommended the steam-blown circulating fluidized bed for future synthesis processes, and corresponding response surfaces for H₂/CO ratio and cold gas efficiency were derived. Overall, Motta et al.³'s research highlights the significant influence of different parameters on syngas composition and overall process performance during sugarcane bagasse gasification.

Begum et al.⁴ investigated an integrated fixed bed gasifier model's performance with different biomass feedstocks using Aspen Plus software. Through Gibbs free energy minimization and validation with experimental data from municipal solid

waste (MSW) and food waste gasification literature, they explored the effects of operating conditions (air-fuel ratio and gasifier temperature) on syngas production for wood, coffee bean husks, green wastes, and municipal solid wastes (MSWs). The researchers found that an air-fuel ratio of 0.3 and gasifier temperature of 700 °C resulted in the best performance for the fixed bed gasifier across all four feedstocks. The model's potential extends to gasification of other biomasses, providing valuable insights into optimal operating conditions for biomass gasification. Therefore, the optimization of the gasification process is crucial to achieve maximum hydrogen production and efficiency.

Gasification is a versatile process that allows the utilization of various gasifying agents in biomass gasification, such as air, steam, oxygen, supercritical water or a combination of these, to efficiently convert biomass into valuable syngas. In conventional biomass gasification, steam is commonly used as the gasifying agent due to its ability to react with the biomass, producing syngas containing hydrogen. However, there is a growing interest in exploring supercritical water as a potential replacement for steam to produce hydrogen, as supercritical water offers higher temperatures and pressures, leading to more efficient gasification reactions and increased hydrogen yields, making it a promising option for hydrogen production from biomass. Researchers^{5,6} are keenly interested in both steam and supercritical water as gasifying agents in biomass gasification due to their unique properties. Steam gasification is well-established and widely used, offering moderate temperatures and pressures, facilitating the production of syngas for various applications. On the other hand, supercritical water gasification, operating at higher temperatures and pressures beyond its critical point, shows great promise in achieving higher gas yields, increased efficiency, and hydrogen-rich syngas, making it an attractive alternative for sustainable hydrogen production from biomass. Comparatively, while steam gasification is more mature and widely adopted, supercritical water gasification holds potential for more

efficient and hydrogen-enriched syngas generation, thereby offering a more sustainable pathway for biomass utilization in hydrogen production. Further research and development will be essential to fully understand and harness the benefits of both techniques in various applications.

Carbon capture is an essential part of hydrogen production from biomass, as the carbon dioxide produced during gasification must be captured to prevent it from being released into the atmosphere. There are many ways to capture carbon, but one method that stands out is calcium oxide (CaO) adsorption. This uses a solid material as CaO to capture carbon dioxide. This approach offers several benefits, including cost-effectiveness, wide availability, reusability and non-toxicity. However, it should be noted that an increase in regeneration cycles leads to a reduction in adsorption efficiency.

In this study, Aspen Plus software was used to model the production of green hydrogen from bagasse gasification. Bagasse was chosen as the feedstock for this study because it is a readily available and inexpensive feedstock in Thailand. This study aims to determine the optimal operating conditions of the green hydrogen production through gasification integrated with CaO adsorption for CO₂ capture. The main target of the study was to produce green hydrogen which is hydrogen produced from renewable energy sources with minimal carbon emissions.

1.2 Objectives

1.2.1 To develop a process design for green hydrogen production from bagasse gasification integrated with CaO adsorption.

1.2.2 To investigate the effect of operating conditions of bagasse gasification on hydrogen production.

1.2.3 To analyze the effect of operating conditions of CaO adsorption on hydrogen production.

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1.2.4 To compare the green hydrogen production obtained from integrated process that uses steam and supercritical water as gasifying agent.

1.3 Scopes of work

1.3.1 Design and simulate two processes of green hydrogen production that include steam gasification integrated with CaO adsorption and supercritical water gasification integrated with CaO adsorption by Aspen Plus version 12 simulation software. Bagasse is considered as feedstock in gasification process.

1.3.2 Validate the simulation results with the experimental data from the literature.

1.3.3 Study the effect of operating conditions of steam gasification process on hydrogen production. The parameters are examined as follows:

- gasifier temperature (600 – 1200 °C)
- gasifier pressure (1 – 15 bar)
- steam to biomass mass ratio (0.1 – 2.0)

1.3.4 Study the effect of operating conditions of supercritical water gasification process on hydrogen production. The parameters are examined as follows:

- gasifier temperature (375 – 1200 °C)
- gasifier pressure (221 – 350 bar)
- steam to biomass mass ratio (0.1 – 2.0)

1.3.5 Study the effect of operating conditions of water gas shift process on hydrogen production in both steam and supercritical water gasification. The parameters are examined as follows:

- water gas shift reactor temperature (150 – 400 °C)
- water to biomass mass ratio (0.1 – 1.5)

1.3.6 Study the effect of operating conditions of CaO adsorption on hydrogen production in both steam and supercritical water gasification. The parameters are examined as follows:

- Carbonator temperature (650 – 850 °C)
- Calcium oxide to biomass mass ratio (0.1 – 2.5)
- Regenerator temperature (400 – 1400 °C)

1.4 Expected outputs

1.4.1 The process model of green hydrogen production produced from bagasse gasification integrated with CaO adsorption can be obtained and used by other researchers.

1.4.2 The optimal operating conditions of green hydrogen production can be provided. The obtained results can be guideline for green hydrogen production from bagasse gasification integrated with CaO adsorption.

CHAPTER II

LITERATURE REVIEW

2.1 Biomass

Biomass⁷ is any type of organic matter that is a natural reservoir of solar energy⁸ and can be used to produce energy. Not counting the conversion to fossil fuels. They are usually made from waste or agricultural residues or from industrial processes such as rice husks, rice straw, bagasse, leaves and tops of sugar cane, wood chips, fibers and palm shells, cassava pulp, corn cobs, husks and coconut shells, solid waste or even animal manure. It is an alternative energy source, which has been widely discussed today because it is renewable all the time. It is not used up like fuel such as oil, natural gas, or coal. Biomass electric power is an alternative to using biomass as a fuel for production.

2.2 Biomass energy

Biomass energy⁹ is the energy produced by using biomass or organic materials of all forms as natural energy storage sources such as organic waste, agricultural waste, residues from industrial processes, animal manure, fuel crops such as rice husks, rice straw, bagasse, sugarcane leaves and shoots, wood, wood chips, fibers and palm shells, cassava pulp, corn cobs, husks and coconut shells come through processing such as fermentation, combustion, gasification or other processes until it is heat or gas to be utilized or converted into electrical energy.

2.3 Advantages of bioenergy/biomass

2.3.1 It can be produced from a wide range of raw materials and can be used in a variety of applications.

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- 2.3.2 It is a renewable energy that can be produced indefinitely and never run out like fossil energy. Including not negatively impacting the environment like fossil energy.
- 2.3.3 It helps reduce the amount of waste and bio-waste generated in households and industries while helping to reduce landfill waste.
- 2.3.4 It is cheaper compared to using fossil energy.
- 2.3.5 Suitable for agricultural countries. This is because it adds value to agricultural waste and increases income for farmers, helping to develop the basic economy.
- 2.3.6 The remaining products in the production process can be used to make organic fertilizers and compost to bring back to use in agriculture.

2.4 Disadvantages of bioenergy/biomass

- 2.4.1 The technology and equipment used to produce high-quality production are still quite expensive. Especially bioenergy that needs expertise in raw material management.
- 2.4.2 Some biomass energy also generates carbon dioxide and fumes in production.
- 2.4.3 Some agricultural raw materials have short shelf life, and some have seasonal production cycles. Therefore, the volume may be uneven at certain times.
- 2.4.4 A large amount of land is needed to produce energy as well as to store raw materials from agricultural crops.

2.5 Process of transforming biomass into various forms of energy¹⁰

2.5.1 Combustion

When biomass is burned. The heat will be released according to the calorific value of the biomass type. The heat obtained by incineration can be

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used to produce steam at high temperatures and pressures. This steam is then used to drive steam turbines to generate electricity. Examples of this type of biomass are agricultural waste and wood chips.

2.5.2 Gasification

Gasification is the process of converting solid fuels or biomass into fuel gas called biogas, consisting of methane, hydrogen and carbon monoxide which can be used for gas turbines.

2.5.3 Fermentation

Fermentation is the use of biomass to ferment with bacteria in anaerobic conditions. Biomass will be decomposed and broken down. It produces biogas that is composed of methane and carbon dioxide. Methane gas is used as a fuel in engines for generating electricity.

2.5.4 Production of liquid fuels from plants with the following production processes:

- Biological processes will decompose starch, sugar, and cellulose from agricultural plants such as sugarcane and cassava into ethanol to be used as liquid fuel in gasoline engines.
- Physics and chemical processes by extracting oil from oil plants and then transferring the oil to the process of transesterification to produce biodiesel.
- High heat processes such as pyrolysis process. When agricultural materials are highly heated in anaerobic conditions, they decompose into fuel in the form of liquid and gas mixed together.

2.6 Bagasse

Bagasse¹¹ is the remnants of sugarcane stalks, which are a fiber that has been crushed to remove sugar cane juice or sugar from sugarcane. It is agricultural waste from the sugar industry. Each year, there is a large amount of bagasse left from the production process. Bagasse is an agricultural biomaterial composed mainly of organic matter. They are high in carbon and cellulose (55% and 48.5% respectively) and are biodegradable by microorganisms.

Advantages of bagasse¹²

- Used as a fuel for electricity generation. Bagasse is a by-product of the sugarcane crushing process. The bagasse has flammable properties. It consists of the main elements: Carbon, Hydrogen, Oxygen and Nitrogen. It has a low heating value, suitable for use as a fuel for power generation.
- Used to produce construction materials mixed with adhesives such as particle board, fiber-overlaid plywood, and insulation board, etc.
- Used to make food packaging. The packaging made from bagasse pulp is a packaging that is friendly to users and the environment.
- Used as animal feed. By fermenting bagasse before feeding animals.
- Biochar can be produced using thermal chemistry from organic raw materials. Bagasse is another good raw material due to its high carbon content, which is currently being used in many fields, including increasing soil fertility use as fuel, use as absorbent material and carbon storage, etc.
- Used to make compost. It uses bagasse to compost together with manure, sludge, or scientific fertilizer; to support animal manure and continue to make compost.
- Use as mulch to maintain soil moisture and prevent weeds.

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2.7 Gasification process

Gasification⁷ is the process of converting biomass into producer gas. Partial oxidation of biomass with steam (H₂O), oxygen (O₂) or air. The reactor is called gasifier. The resulting fuel gas has a different composition depending on the type and properties of the biomass used as the reactant. The main components of fuel gas include carbon monoxide (CO) and hydrogen (H₂), which may contain some methane (CH₄) and carbon dioxide (CO₂). Other products are also obtained, such as tar and ash. The gasification process in the gasifier is divided into 4 zones¹³ as follows:

2.7.1 Drying zone

It is the zone at the top that is responsible for drying and evaporating the water from the raw materials by heat. In the temperature range from about 40-200 °C, at such temperature, the humidity can be reduced by about 5% and the moisture content of raw materials suitable for use should be lower than 30 percent in order for the fuel raw materials to have dryness and easy to ignite.

2.7.2 Devolatilization zone or Pyrolysis zone

It is a zone that is attached to the combustion zone and is directly heated by the combustion zone by devolatilization or pyrolysis, where charcoal, gas, byproducts and tar are obtained. The reactions occur in the temperature range of about 500-600 °C.

2.7.3 Combustion zone

In the gasifier furnace, there is a special area that generates heat and sends it to other parts. This zone is where a reaction happens that involves burning the raw material or carbon from another area to create both carbon dioxide and heat. The heat produced is then sent directly to the reduction and pyrolysis sections, as well as the drying area.

2.7.4 Reduction zone

It is a zone that produces syngas. It contains carbon monoxide and hydrogen as the main products. By the process of converting carbon into syngas, the reaction takes place in the temperature range of about 800-1000 °C of combustion under air-limiting conditions, which will break up the carbon and tar into syngas.

2.8 Syngas

Synthesis gas¹⁴, also known as syngas, is a term for a gas product developed from the synthesis of hydrogen and carbon monoxide by several production methods. Some of the methods used to produce syngas include coal gasification, natural gas steam reforming, waste to energy and biomass power generation. Syngas is also an intermediate by-product developed during the processing of ammonia, methanol, synthetic petroleum, or synthetic natural gas. Syngas can be used as a lubricant or fuel.

Syngas is often used to generate steam and electricity and is a chemical ingredient in the petrochemical refining business. Petroleum byproducts that may become waste can be preserved as raw materials for production. These materials react under greatly elevated pressure and temperature in the reactor to produce syngas. During gasification, any material containing carbon can be converted. Biomass production is the most commonly used method in syngas production.

The lower heating value (LHV) refers to the heat value that is released after complete combustion when the water contained in the fuel and produced by combustion is in the form of steam. The lower heating value is important for syngas production as it enables the optimization of process parameters, influences product quality, and has implications for energy efficiency and economic considerations. The

calculation of the lower heating value (LHV), which is an important consideration in the production of synthesis gas, can be expressed as Equation (2-1)¹⁵.

$$\text{LHV} = 12.60 \text{ CO} + 10.79 \text{ H}_2 + 35.87 \text{ CH}_4 \quad (2-1)$$

where LHV is lower heating value (MJ/Nm³), CO is mole fraction of carbon monoxide, H₂ is mole fraction of hydrogen and CH₄ is mole fraction of methane.

2.9 Supercritical water

Supercritical water¹⁶ is a state of water that exists at temperatures and pressures above its critical point, which temperature is approximately 374 °C and pressure is approximately 221 bar (or 22.1 MPa). At this point, water undergoes a phase transition and becomes a supercritical fluid with properties of both a liquid and a gas.

Supercritical water is characterized by its unique properties, including high density, low viscosity, and high diffusivity, which make it useful for a variety of industrial applications. It is used in the production of biofuels, as a solvent for chemical reactions, and as a coolant in nuclear reactors, among other applications. Supercritical water is also being researched as a potential method for waste treatment and destruction, as it can break down organic materials to their basic components through oxidation.

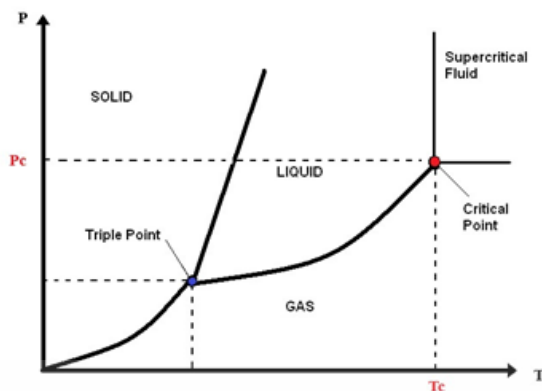


Figure 2.1 Schematic diagram phase of water.

2.10 CO₂ capture process

Currently, there are various methods to capture carbon dioxide gas, including the use of liquid absorbents, membrane separation, reducing temperature to condense carbon dioxide gas into a liquid, and the use of solid adsorbents. This research will specifically explain the technology of carbon dioxide capture using the solid adsorption¹⁷ of calcium oxide (CaO).

The process of carbon dioxide capture by calcium oxide adsorption is one method of capturing carbon dioxide. In this process, carbon dioxide is passed through the calcium oxide adsorption unit, and a reaction between calcium oxide and carbon dioxide occurs, called "carbonation." This results in the formation of calcium carbonate (CaCO₃).

This process is called "CaO adsorption" and is an effective method of capturing carbon dioxide. Calcium oxide can be reused multiple times and the carbon dioxide that is adsorbed can be used in further processes. Calcium carbonate can be broken down by heat, called "calcination," to produce carbon dioxide and calcium oxide, which can then be reused in the adsorption process.

2.11 Literature review

Motta et al.¹⁸ aims to simulate and analyze different operating parameters, fluidizing media, and gasifier types for sugarcane bagasse gasification. Sugarcane bagasse gasification is a thermochemical process that converts sugarcane residue (bagasse) into syngas, which can be used to generate heat, electricity, and liquid fuels. The study analyzes the influence of various operational parameters such as temperature, pressure, steam to biomass mass ratio (S/B), and moisture content on syngas composition and process performance. The fluidized bed configurations (bubbling and circulating) and gasifying media (steam and steam-oxygen) were also studied. The results show that temperature is crucial for higher hydrogen and carbon monoxide production, CO₂ consumption, higher syngas lower heating value (LHV), and higher cold gas efficiency (CGE). Among the gasifier configurations, the circulating fluidized bed was recommended for future synthesis processes, since it led to higher hydrogen and carbon monoxide generation, lower carbon dioxide and methane production.

Shahbaz et al.¹⁹ presents a simulation model of steam gasification of palm kernel shell (PKS) with CO₂ capture through CaO sorbent using Aspen plus. The objective of the study was to investigate the effect of key parameters like temperature, steam/biomass ratio, and CaO to biomass ratio on syngas yield. The simulation results showed that the hydrogen concentration increased from 65 to 79.32 vol % with the increase of temperature from 650 to 700 °C. The CO₂ content was reduced from 20 to 5.32 vol % by increasing the CaO to biomass ratio from 0.5 to 1.42. The maximum hydrogen content predicted is 79.32 vol %, and the minimum carbon dioxide content is 5.42 vol % found at operating parameters including a temperature of 700 °C, steam/biomass ratio of 1.5, and CaO to biomass ratio of 1.42. The system performance was evaluated through carbon conversion efficiency, cold gas efficiency and gasification efficiency, lower and higher heating values by varying

the gasification temperature, steam to biomass ratio, and CaO to biomass ratio. The simulation model predicted results were compared with experimental data obtained from the experimental set up used in the simulation.

Li et al.²⁰ studied the effect of adding absorbents (such as CaO) for in-situ CO₂ removal during the steam gasification process of biomass to produce more hydrogen. A model of calcium oxide enhanced steam gasification of biomass for hydrogen production was built using Aspen Plus software. The results showed that increasing the molar ratio of calcium to carbon and the steam to biomass ratio can increase the hydrogen concentration and production, while higher pressure (>0.6 MPa) is not favorable for hydrogen formation. The suitable condition for hydrogen production is at a gasification temperature of 600-700 °C, with atmospheric pressure or slight pressurization (≤ 0.6 MPa), and the molar ratio of calcium to carbon should be greater than or equal to the carbon conversion rate.

CHAPTER III

RESEARCH METHODOLOGY

In this chapter, the process description of green hydrogen production from bagasse gasification integrated with CaO adsorption is presented. Section 3.1 presents the process overview of hydrogen production from steam and supercritical water gasification of bagasse integrated with CaO adsorption. Next, the process models of hydrogen production from steam and supercritical water gasification of bagasse are described Section 3.2. Section 3.3 explains the process model of CaO adsorption for CO₂ capture. While Section 3.4 provides an overview of the simulation approach.

3.1 Process overview of hydrogen production from bagasse gasification integrated with CaO adsorption

The process flow diagrams of hydrogen production from bagasse through steam gasification integrated with CaO adsorption (SG-CaO) and supercritical water gasification integrated with CaO adsorption (SCWG-CaO) are demonstrated in Figures 3.1 and 3.2. Both processes consist of three parts. The first part involves bagasse gasification, wherein syngas is produced through the gasification process using a gasifying agent like steam or supercritical water. The primary objective of this project is to generate hydrogen; hence, the obtained syngas from bagasse gasification undergoes improvement in the second part, known as the water gas shift process. In this step, carbon monoxide is converted to hydrogen and carbon dioxide. Finally, the syngas is delivered to the third part, the CaO adsorption process, where carbon dioxide is captured using calcium oxide, resulting in the production of green hydrogen.

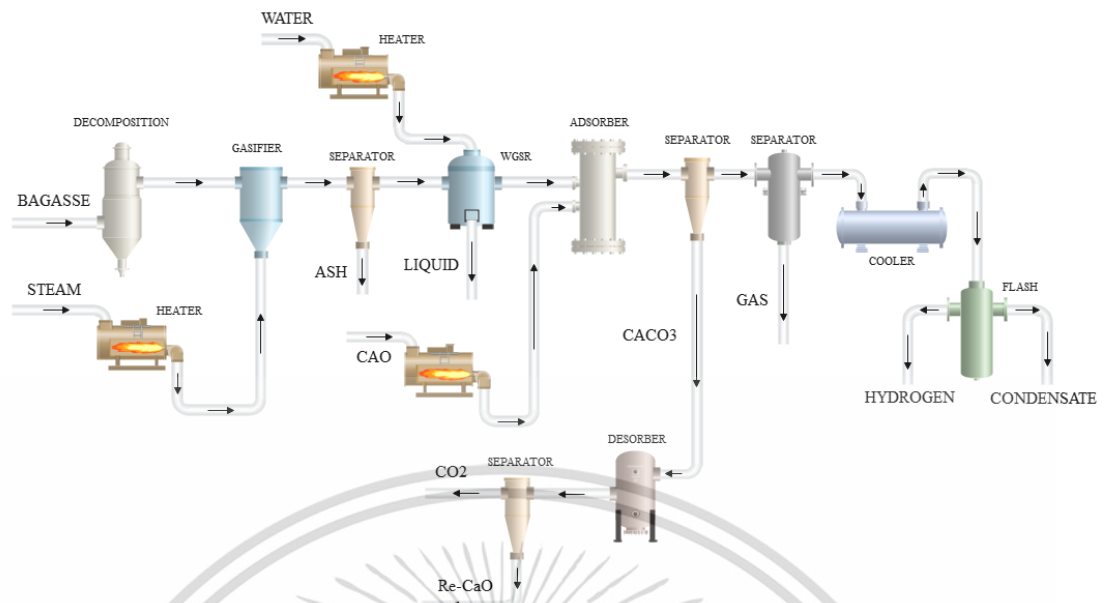


Figure 3.1 Process flow diagram of hydrogen production from bagasse through steam gasification integrated with CaO adsorption (SG-CaO)

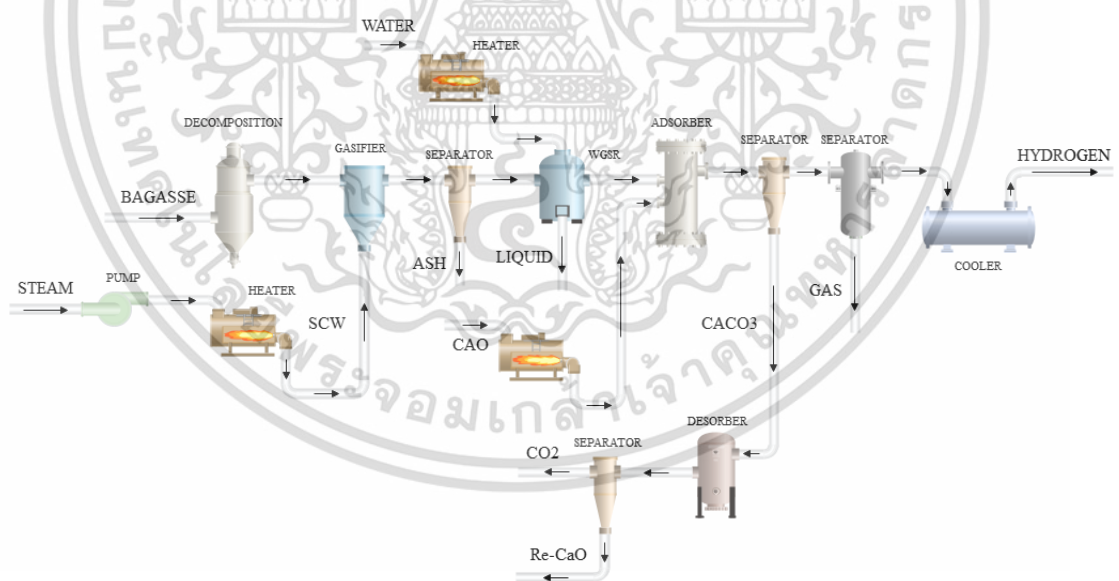


Figure 3.2 Process flow diagram of hydrogen production from bagasse through supercritical water gasification integrated with CaO adsorption (SCWG-CaO)

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3.2 Process model of hydrogen production from bagasse gasification

The flowsheet of the steam gasification and supercritical water gasification processes designed in Aspen Plus version 12 simulation software are illustrated in Figures 3.3 and Figure 3.4, respectively. Bagasse is utilized as a feedstock. In this project, the non-conventional components of biomass are specified in the Aspen Plus simulator, and the ultimate and proximate analysis of bagasse as presented in Table 3.1 are defined in the simulation. The devolatilization of biomass is carried out in the decomposition unit (DECOMP), converting non-conventional components (BAGASSE stream) into conventional components (INGASIF stream). Then, INGASIF stream is transferred to the gasification unit (GASIF). The gasification unit utilizes a gasifying agent, which can be steam (STEAM2 stream) or supercritical water (SCW stream), to react with the biomass.

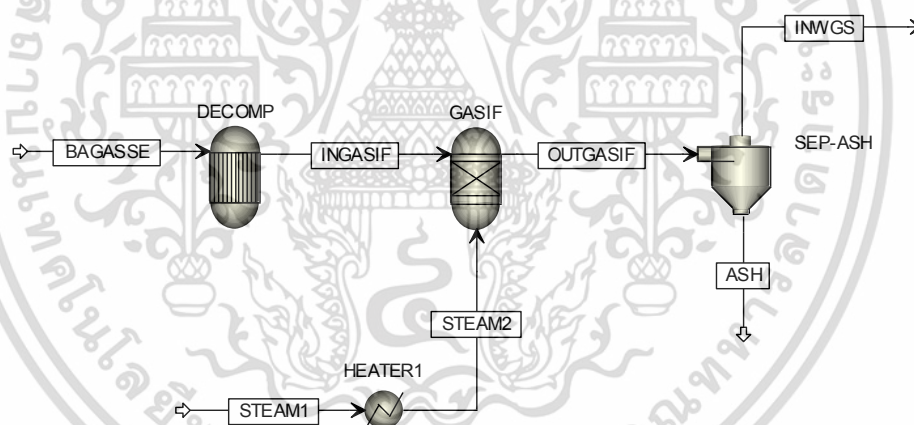


Figure 3.3 Flowsheet of hydrogen production from steam gasification of bagasse.

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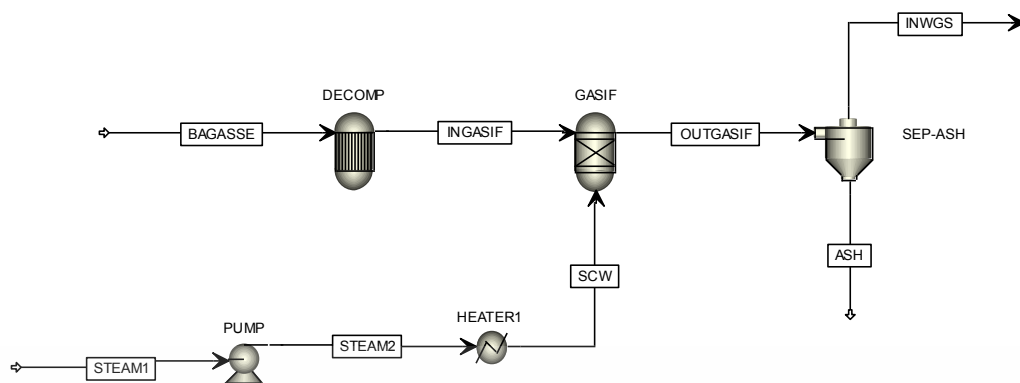


Figure 3.4 Flowsheet of hydrogen production from SCW gasification of bagasse.

Table 3.1 Ultimate and proximate analysis of bagasse²¹

Ultimate Analysis	Composition (%)
Carbon	49.80
Hydrogen	6.00
Oxygen	43.90
Nitrogen	0.20
Chlorine	0.04
Sulphur	0.06
Proximate Analysis	Composition (%)
Moisture	10.4
Volatile matter	76.6
Fixed Carbon	11.1
Ash	1.9

In the case of steam gasification, a heater (HEATER1) must be installed to increase the temperature of the steam prior to entering the gasification unit.

Conversely, if supercritical water (SCW) is used as the gasifying agent, both a pump

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(PUMP) and heater (HEATER1) must be installed to increase the pressure and temperature of the water, respectively, before entering the gasification unit (GASIF). Many possible of chemical reactions can be taken place, as described below:

Char partial combustion:



C combustion:



CO partial combustion:



Methane combustion:



H₂ partial combustion:



Boudouard reaction:



Water gas reaction:



Hydrogenation reaction:



Water gas shift reaction:



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Methanation reaction:



Reforming reaction:



The gas obtained from bagasse gasification (OUTGASIF stream) consists of hydrogen, carbon monoxide, carbon dioxide, other gases, and ash. The ash can be further removed through a cyclone (SEP-ASH). Since the gas product in the INWGS stream contains a high amount of carbon monoxide, it is necessary to install a water gas shift reactor to convert the carbon monoxide into more carbon dioxide and hydrogen by introducing water into the process. Figure 3.5 illustrates a diagram of installation of water gas shift reactor in both steam and supercritical water gasification. From Figure 3.5, the WATER stream was heated by heater (HEATER2) before entering water gas shift reactor (WGS), where the water gas shift reaction (Eq. (3-9)) occurs. As a result, an INADSORB stream with a reduced amount of carbon monoxide is obtained from the water gas shift reactor. In order to obtain pure hydrogen, it is necessary to remove the carbon dioxide from the gas mixture, which can be achieved through adsorption, using calcium oxide (CaO) as an adsorbent.

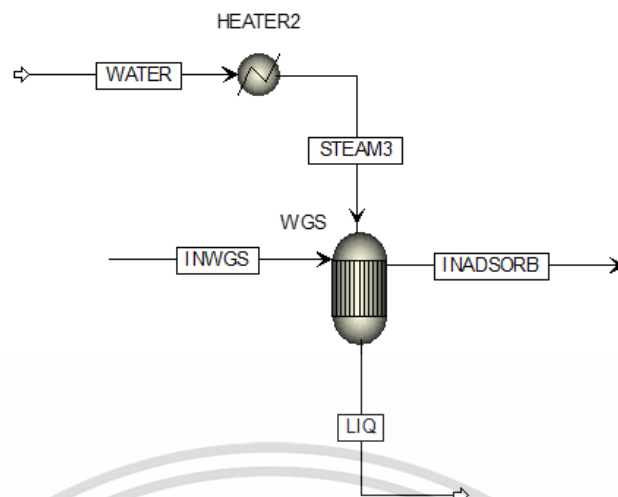


Figure 3.5 Diagram of installation of water gas shift reactor
(Both steam and supercritical water gasification).

3.2.1 Validation of simulation results with experimental data

In order to verify the efficacy of the proposed Aspen Plus simulation process model, the simulation results of gasification were validated by comparing with experimental data of Loha et al.²². Rice husk was the feedstock utilized in their steam gasification experiment. The ultimate and proximate analysis of rice husk used in their experiment is shown in Table 3.2. In their experiment, the gasifier was operated at a temperature of 750 °C and a pressure of 1 bar, with a steam to biomass mass ratio of 1.

Additionally, Wang et al.⁵ performed supercritical water gasification from wheat straw in which the ultimate and proximate analysis data are provided in Table 3.3. The gasifier used in their experiment operated at a temperature of 750 °C and pressure of 230 bar and supercritical water to biomass mass ratio of 1.

Table 3.2 Ultimate and proximate analysis of rice husk for steam gasification²³

Ultimate Analysis	Composition (%)
Carbon	38.43
Hydrogen	2.97
Oxygen	36.36
Nitrogen	0.49
Sulphur	0.07
Ash	21.68
Proximate Analysis	Composition (%)
Volatile matter	55.54
Fixed Carbon	14.99
Ash	19.52
Moisture	9.95

Table 3.3 Ultimate and proximate analysis of wheat straw for SCW gasification⁵

Ultimate Analysis	Composition (%)
Carbon	38.43
Hydrogen	2.97
Oxygen	36.36
Nitrogen	0.49
Sulphur	0.07
Ash	21.68
Proximate Analysis	Composition (%)
Volatile matter	55.54
Fixed Carbon	14.99
Ash	19.52
Moisture	9.95

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3.2.2 Investigation on effect of operating conditions in bagasse gasification

In this section, both steam gasification and supercritical water gasification of bagasse were examined to analyze the effects of key gasification parameters including gasifier temperature, gasifier pressure, and gasifying agent (steam or supercritical water) to biomass mass ratio on the production of hydrogen. The parameters for steam gasification process are shown in Table 3.4 while Table 3.5 presents the parameters for the supercritical water gasification process.

Table 3.4 Parameters and operating conditions of steam gasification of bagasse

Parameter	Operating condition
Gasifier temperature (°C)	600 – 1200
Gasifier pressure (bar)	1 – 15
Steam to biomass mass ratio	0.1 - 2.0

Table 3.5 Parameters and operating conditions of supercritical water gasification of bagasse

Parameter	Operating condition
Gasifier temperature (°C)	375 – 1200
Gasifier pressure (bar)	221 – 350
Supercritical water to biomass mass ratio	0.1 - 2.0

3.2.3 Investigation on effect of operating conditions in water gas shift reactor

In this section, both steam gasification and supercritical water gasification of bagasse were examined to analyze the effects of key water gas shift reactor parameters including water gas shift reactor temperature, and water to biomass mass ratio. The parameters for water gas shift reactor (WGS) are shown in Table 3.6.

Table 3.6 Parameters and operating conditions of water gas shift reactor (WGS)

Parameter	Operating condition
Water gas shift reactor temperature (°C)	150 - 400
Water to biomass mass ratio	0.1 – 1.5

3.3 Process model of CaO adsorption for CO₂ capture

Figures 3.6 and 3.7 illustrate a diagram of CaO adsorption integrated in steam and supercritical water gasification, respectively. In the CaO adsorption unit, the INADSORB stream obtained from the water gas shift unit is reacted with calcium oxide (CAO stream) in the adsorber unit (ADSORBER). Inside this unit, a carbonation reaction (Eq. (3-14)) takes place between carbon dioxide and calcium oxide, resulting in the formation of solid calcium carbonate. The OUTADSOR stream contains calcium carbonate, hydrogen, and other components, which is then directed to the separator (SEP-1). The separator is responsible for separating the solid calcium carbonate from the gases. The separated calcium carbonate is referred to as the CaCO₃ stream, while the gases are represented with the LEAN-CO₂ stream.

The CaCO_3 stream is sent to the regenerator (DESORBER), where a calcination reaction (Eq. (3-15)) takes place, causing the calcium carbonate to break down into carbon dioxide and calcium oxide. This process enables the calcium oxide to be reused in future adsorption processes.

Carbonation reaction:



Calcination reaction:

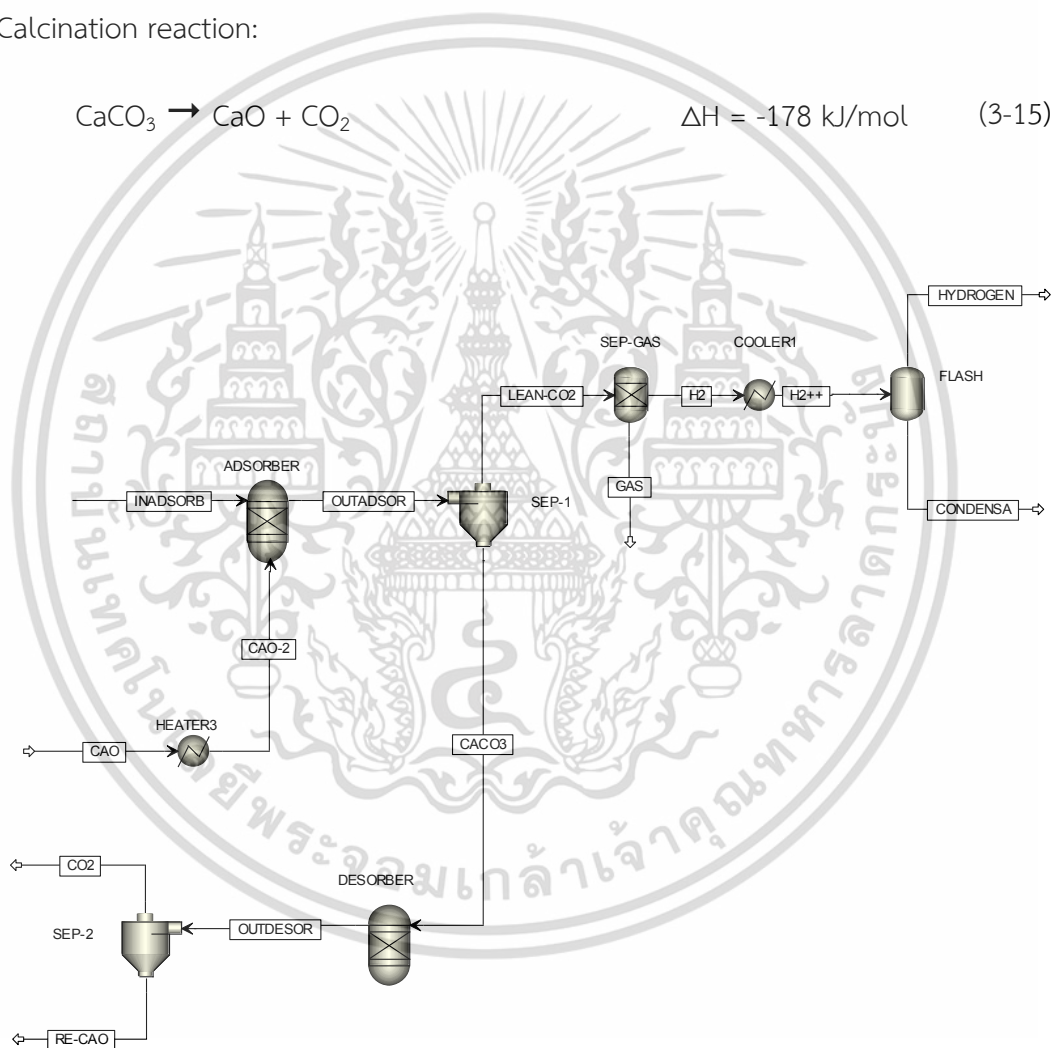


Figure 3.6 Diagram of CaO adsorption (Steam gasification).

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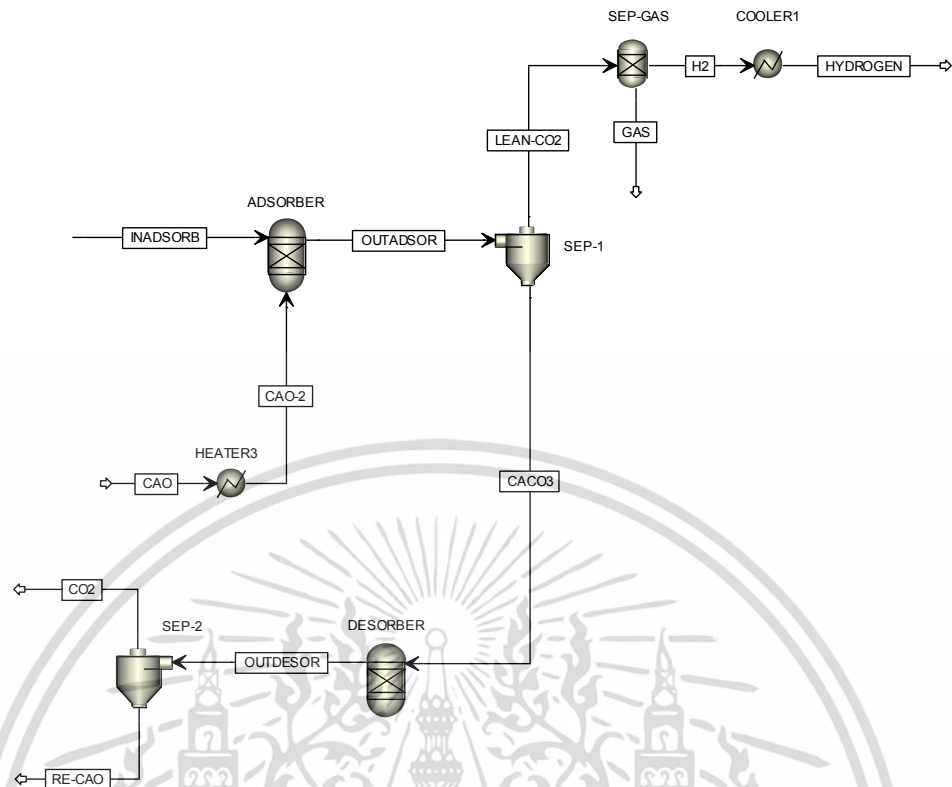


Figure 3.7 Diagram of CaO adsorption (Supercritical water gasification).

The LEAN-CO₂ stream is directed to the gas separator (SEP-GAS) for the purpose of separating the hydrogen (H₂ stream) from other gases (GAS stream). The H₂ stream is cooled to reduce its temperature. If steam gasification is employed (Figure 3.6), a flash separator (FLASH) is necessary to separate water from hydrogen. However, in the case of supercritical water gasification (Figure 3.7), no additional equipment is required. As a result, the HYDROGEN stream achieves the highest level of purity.

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3.3.1 Investigation on effect of operating conditions in CaO adsorption on hydrogen production

In CaO adsorption unit, the impact of key parameters such as calcium oxide to biomass mass ratio, carbonator temperature (ADSORBER), and regenerator temperature (DESORBER) on the production of hydrogen during CaO adsorption were analyzed. The parameters relevant to both steam and supercritical water gasification are considered in Table 3.7.

Table 3.7 Parameters and operating conditions of CaO adsorption

Parameter	Operating condition
Carbonator temperature (°C)	650 – 850
Calcium oxide to biomass mass ratio	0.1 – 2.5
Regenerator temperature (°C)	400 – 1400

Based on the studies, the optimal operational parameters for bagasse gasification integrated with CaO adsorption have been determined, leading to the accomplishment of the highest purity in hydrogen production.

3.4 Simulation approach

Figures 3.8 and 3.9 present the green hydrogen production process from the integration of bagasse gasification and CaO adsorption with different gasifying agents. The simulation of green hydrogen production process is performed through Aspen Plus version 12 simulation software. The Peng-Robinson with Boston-Mathias modifications²⁴ is selected as equation of state since the chosen property method is capable of delivering reliable and accurate results across a wide range of temperatures and pressures, exhibiting consistency especially in the critical region. In order to determine the physical properties of non-conventional biomass components, enthalpy and density, HCOALGEN and DCOALIGT are crucial parameters that are used for calculation.

Firstly, the composition of bagasse is defined as indicated in Table 3.1. In the study of the SG-CaO process, the operating conditions for gasification, water gas shift reactor, and CaO adsorption are defined as shown in Table 3.8. In the case of the SCWG-CaO process, the operating conditions are defined according to Table 3.9. The equilibrium gas compositions during the gasification process are determined using the minimum Gibbs free energy method. When the gas product obtained from gasification process is introduced to water gas shift reactor and CaO adsorption process, the green hydrogen can be provided as reported in HYDROGEN stream.

In this work, two integrated processes for hydrogen production are considered, namely SG -CaO and SCWG-CaO process. To determine the appropriate process for green hydrogen production, not only the quality and quantity of hydrogen are determined, but also the carbon dioxide emissions are considered. When the optimal operating conditions for both processes are determined, the energy analysis is performed. The energy efficiency can be calculated using the following equation.

$$\eta_{H_2} = \frac{m_{H_2} \times LHV_{H_2} + Q_{output}}{m_{biomass} \times LHV_{biomass} + Q_{input}} \quad (3-16)$$

where

η_{H_2} represents the overall efficiency of the process, expressed as a percentage (%).

m_{H_2} represents the mass flow rate of hydrogen, measured in kilograms per hour (kg/hr).

LHV_{H_2} stands for the lower heating value of hydrogen, measured in kilojoules per kilogram (kJ/kg).

$m_{biomass}$ represents the mass flow rate of biomass, measured in kilograms per hour (kg/hr).

$LHV_{biomass}$ stands for the lower heating value of biomass, measured in kilojoules per kilogram (kJ/kg).

Q_{output} represents the heat duty released from each unit operation, measured in kilojoules per hour (kJ/hr).

Q_{input} represents the heat duty that is input into each unit operation, measured in kilojoules per hour (kJ/hr).

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Table 3.8 Operating condition of each unit models in steam gasification of bagasse integrated with CaO adsorption on hydrogen production.

Unit operation	Unit model	Initial Conditions	Operational range
Gasification			
DECOMP	Reactor (RYield)	700 °C and 1 bar	-
GASIF	Reactor (RGibbs)	700 °C and 1 bar	700 – 1,200 °C 1 – 15 bar
HEATER1	Exchanger (Heater)	150 °C	-
SEP-ASH	Splitter (SSplit)	-	-
Water gas shift reactor			
WGS	Reactor (REquil)	150 °C and 1 bar	150 – 400 °C
HEATER2	Exchanger (Heater)	150 °C	-
CaO adsorption			
ADSORBER	Reactor (RGibbs)	650 °C and 1 bar	650 – 850 °C
HEATER2	Exchanger (Heater)	650 °C	-
DESORBER	Reactor (RGibbs)	900 °C and 1 bar	400 – 1,400 °C
SEP-1	Separator (SEP)	-	-
SEP-2	Separator (SEP)	-	-
SEP-GAS	Separator (SEP)	-	-
COOLER1	Exchanger (Heater)	25 °C	-
FLASH	Separator (Flash2)	20 °C and 50 bar	-

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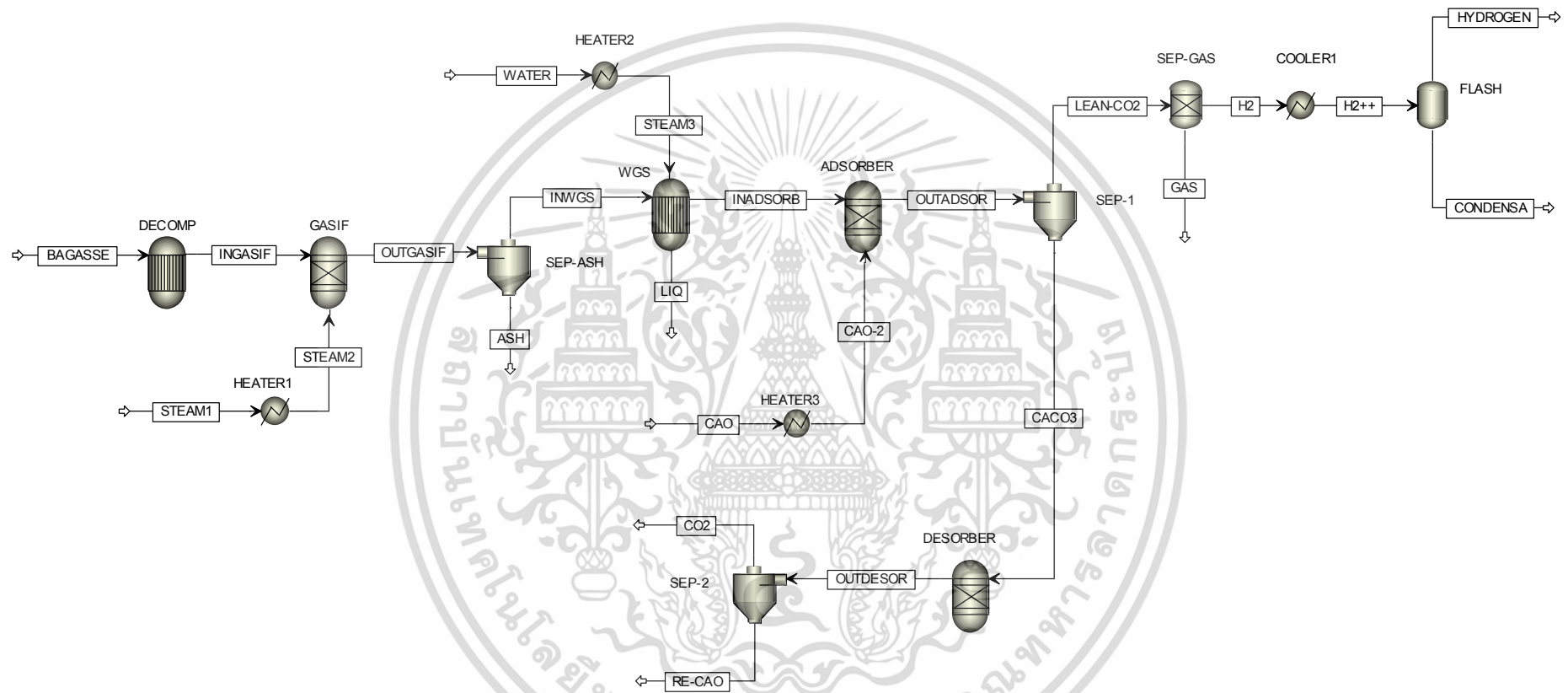


Figure 3.8 Diagram of green hydrogen production from steam gasification of bagasse integrated with CaO adsorption.

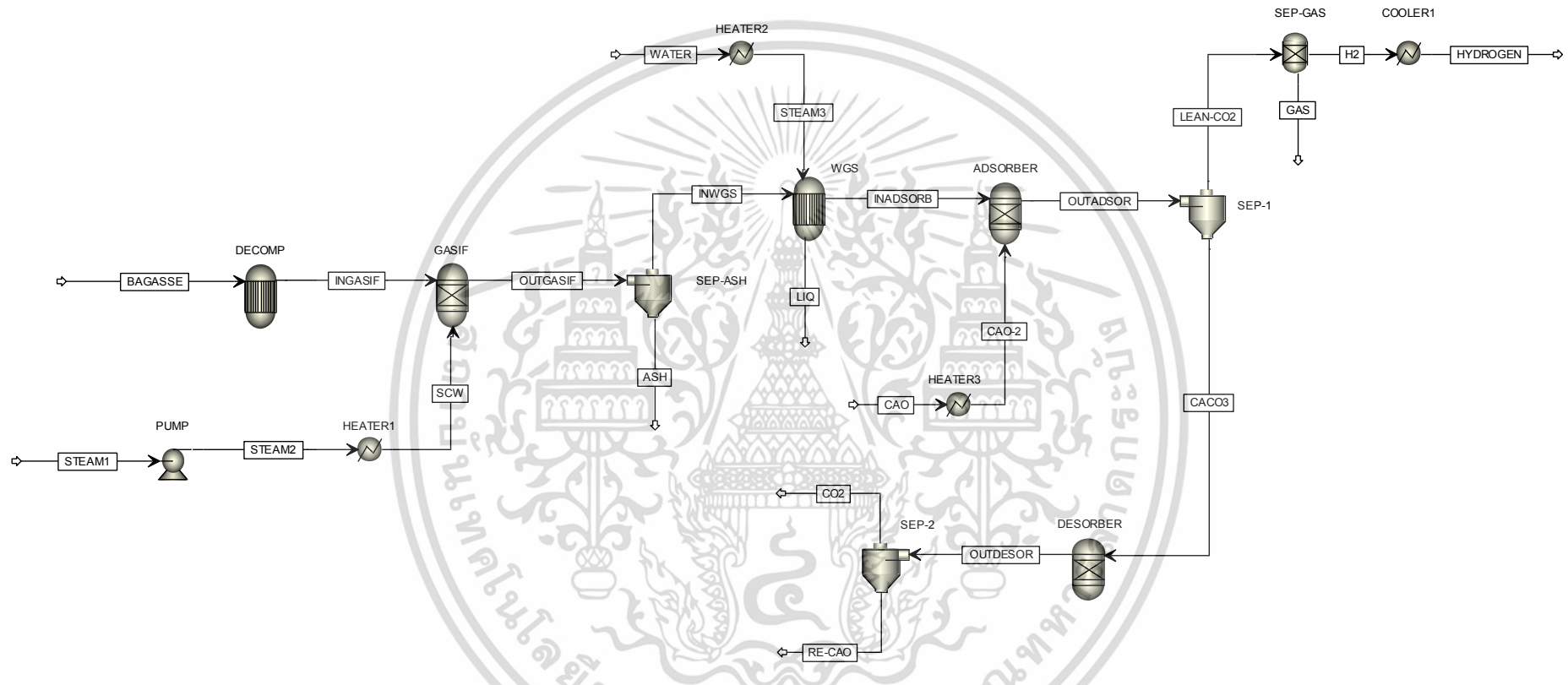


Figure 3.9 Diagram of green hydrogen production from supercritical water gasification of bagasse integrated with CaO adsorption.

Table 3.9 Operating condition of each unit models in supercritical water gasification of bagasse integrated with CaO adsorption on hydrogen production.

Unit operation	Unit model	Initial Conditions	Operational range
Gasification			
DECOMP	Reactor (RYield)	700 °C and 221 bar	-
GASIF	Reactor (RGibbs)	700 °C and 221 bar	700 – 1,200 °C 221 – 350 bar
HEATER1	Exchanger (Heater)	150 °C	-
PUMP	Pressure Changer (Pump)	221 bar	-
SEP-ASH	Splitter (SSplit)	-	-
Water gas shift reactor			
WGS	Reactor (REquil)	150 °C and 1 bar	150 – 400 °C
HEATER2	Exchanger (Heater)	150 °C	-
CaO adsorption			
ADSORBER	Reactor (RGibbs)	650 °C and 1 bar	650 – 850 °C
HEATER2	Exchanger (Heater)	650 °C	-
DESORBER	Reactor (RGibbs)	900 °C and 1 bar	400 – 1,400 °C
SEP-1	Separator (SEP)	-	-
SEP-2	Separator (SEP)	-	-
SEP-GAS	Separator (SEP)	-	-
COOLER1	Exchanger (Heater)	25 °C	-

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CHAPTER IV

STEAM BAGASSE GASIFICATION

This research focuses on the green hydrogen production via bagasse gasification integrated with CaO adsorption process. Two types of gasifying agent, that include steam and supercritical water, are used for hydrogen production. This chapter presents the simulation results of steam bagasse gasification integrated with CaO adsorption. Section 4.1 shows the comparison results of gas product between the simulation results and experimental data of steam gasification of biomass. Section 4.2 discusses the impact of operating conditions in steam gasification on hydrogen production and lower heating value. Section 4.3 presents the effects of operating conditions in water gas shift process while Section 4.4 describes the effect of CaO adsorption operating conditions on hydrogen production. Lastly, the optimal operating conditions in all units and simulation results obtained from this study is summarized in Section 4.5.

4.1 Comparison results between simulation and experiment

In order to verify the efficacy of the proposed Aspen Plus simulation process model, the simulation results of gasification were validated by comparing with experimental data. Rice husk was the feedstock utilized by Loha et al.²² in their steam gasification experiment, as shown in Table 3.2, with their gasifier operating at a temperature of 750 °C and a pressure of 1 bar, with a steam to biomass mass ratio of 1. The comparison results for steam gasification obtained from both the experiment and simulation are presented in Table 4.1. It can be seen that under the same feedstock and same operating condition with the experiment, the simulation results show similar trends to the experimental data. The mean absolute error (MAE) is 5.14, which does not exceed 10 and is an acceptable value. However, it can be observed

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ไม่ว่ากรณีใดๆ ทั้งสิ้น อีกทั้งห้ามมิให้ดัดแปลงเนื้อหา และต้องอ้างอิงถึงเจ้าของเอกสารทุกครั้งที่มีการนำไปใช้

that the methane composition obtained from the simulation is more deviated with the experimental data. The experimental setup may have certain conditions or factors that are difficult to replicate in the simulation, leading to differences in methane production.

Table 4.1 The comparison of syngas production from steam gasification of rice husk between experimental results by Loha et al.²² and simulation results in this study.

Syngas composition (%vol)	Experiment	Simulation
CO	23.7	18.96
CO ₂	21.2	24.32
CH ₄	5.60	0.053
H ₂	49.5	56.67
MAE	5.14	

4.2 Operating conditions in steam gasification

In the first case, steam was employed as the gasifying agent to produce hydrogen through bagasse gasification. This section presents the effects of operating conditions in gasification including gasifier temperature, gasifier pressure and steam to biomass mass ratio on hydrogen production.

4.2.1 Effect of gasifier temperature on hydrogen production

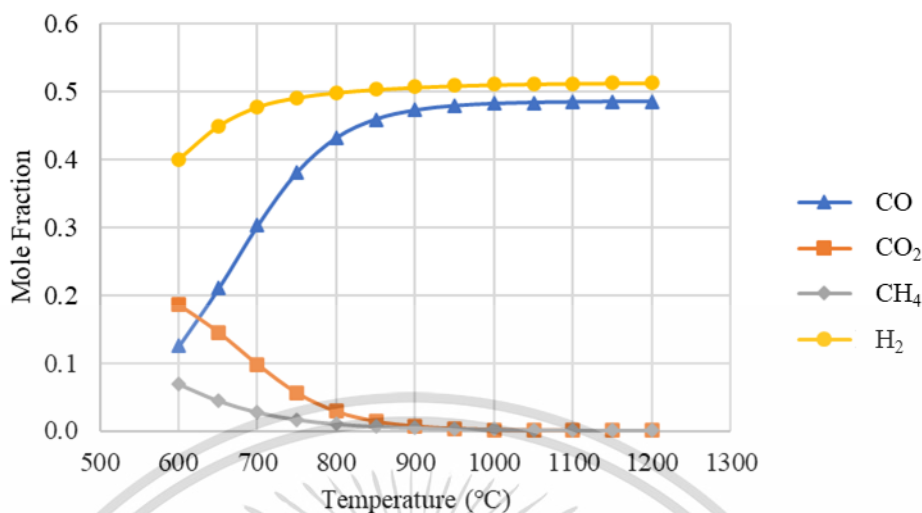


Figure 4.1 Effect of gasifier temperature on hydrogen production at gasifier pressure of 1 bar and steam to biomass mass ratio of 0.1.

In the study, the effect of gasifier temperature on hydrogen production is demonstrated in Figure 4.1, with the gasifier temperature ranging from 600 to 1200 °C while the gasifier pressure and steam to biomass mass ratio are held constant at 1 bar and 0.1, respectively. The results indicate that increasing the gasifier temperature leads to an increase in the mole fraction of carbon monoxide and hydrogen while reducing the mole fraction of carbon dioxide and methane. This is because the high-temperature operation promotes the endothermic reactions, such as Boudouard reaction (Equation (3-6)), water-gas reaction (Equation (3-7)), and reforming reaction (Equation (3-13)), being shifted forward and this results in higher carbon monoxide and hydrogen and lower carbon dioxide and methane. From the simulation results, it is found that the gasifier temperature of 950 °C is identified as the optimum, as it maintains a constantly high mole fraction of hydrogen.

4.2.2 Effect of gasifier pressure on hydrogen production

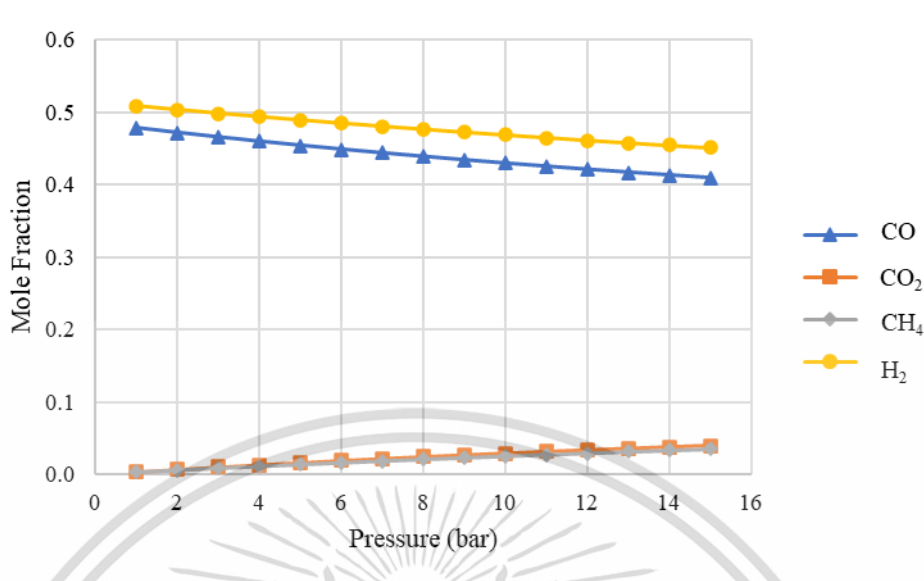
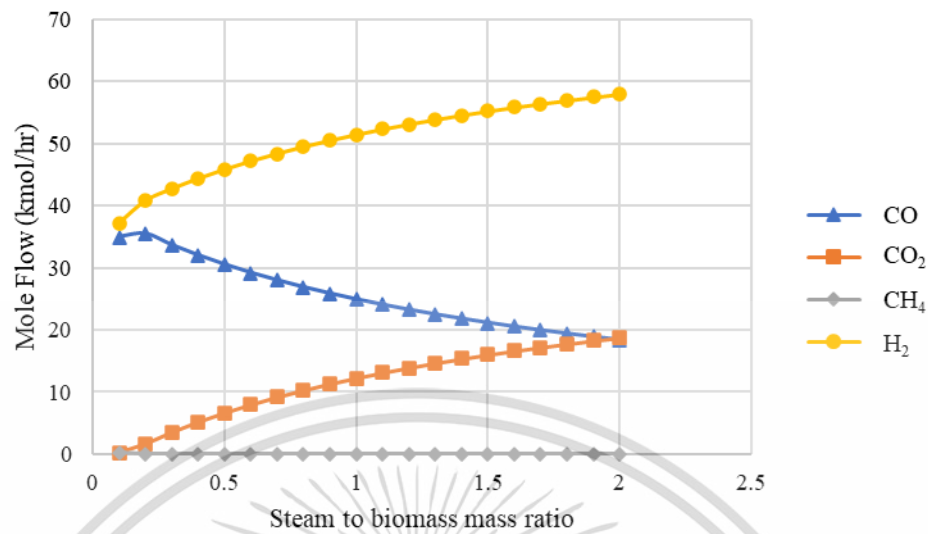


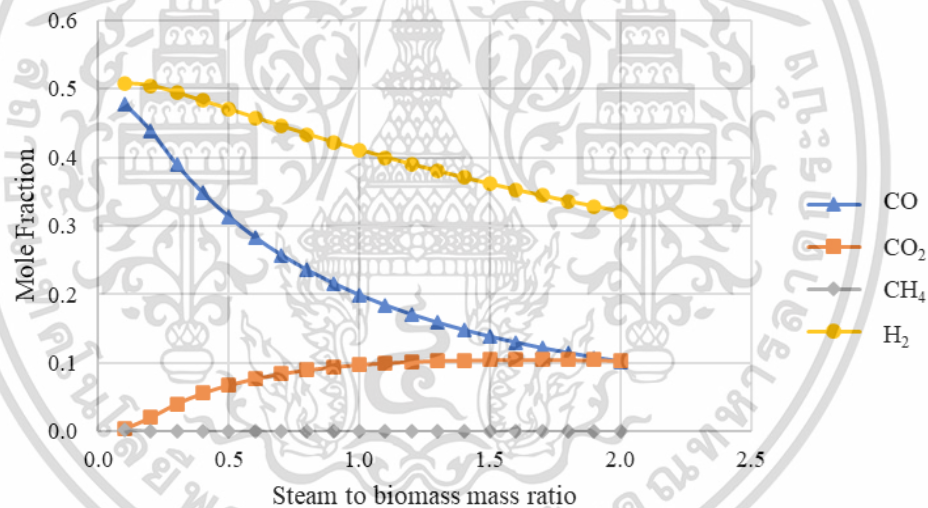
Figure 4.2 Effect of gasifier pressure on hydrogen production at gasifier temperature of 950 °C and steam to biomass mass ratio of 0.1.

The study presented in this section investigates the effect of gasifier pressure on hydrogen production, as illustrated in Figure 4.2, where the gasifier pressure is varied from 1 to 15 bar while maintaining a fixed gasifier temperature and steam to biomass mass ratio at 950 °C and 0.1, respectively. The simulation results show that as gasifier pressure increases, the mole fraction of carbon dioxide and methane also increases, while the mole fraction of carbon monoxide and hydrogen decreases. This can be explained by Le Châtelier's principle, which explains that increasing pressure can shift the chemical equilibrium towards the side with fewer gaseous moles, whereas decreasing pressure can shift the equilibrium towards the side with more gaseous moles. After analyzing the chemical reactions involved in gasification, specifically Equations (3-1), (3-8), (3-10), (3-11), (3-12), and (3-13), it was discovered that the number of moles on the reactant side is greater than that on the product side, indicating that the reaction will proceed forward. Based on the simulation results, it is recommended to operate the gasifier at pressure of 1 bar to maintain high mole fraction of hydrogen.

4.2.3 Effect of steam to biomass mass ratio on hydrogen production



a) Molar flow rate of gas product



(b) Mole fraction of gas product

Figure 4.3 Effect of steam to biomass mass ratio on (a) molar flow rate of gas product and (b) mole fraction of gas product at gasifier temperature of 950 °C and gasifier pressure of 1 bar.

In this study, the effect of steam to biomass mass ratio on hydrogen production was analyzed and presented in Figure 4.3. This study focuses on a range of ratios

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between 0.1 to 2, with the gasifier operating at temperature of 950°C and pressure of 1 bar. Figure 4.3(a) shows the effect of steam to biomass mass ratio on molar flow rate of gas product. The results reveal that adding more steam relative to biomass can increase the production of hydrogen. This is because extra steam encourages the reforming reaction (Equation (3-13)) and water gas shift reactions (Equation (3-9)) to produce more hydrogen. As a result, the amount of carbon monoxide in the reforming process decreases. It is also noticed that adding more steam makes the resulting reformat gas, which contains carbon monoxide, less concentrated.

However, the result shown in Figure 4.3(b) is evident that as the steam to biomass mass ratio rises, the mole fraction of carbon dioxide increases, while the mole fraction of hydrogen, carbon monoxide, and methane decline due to the added steam in the gasification process. This shift in equilibrium for water gas reaction (Equation (3-7)), water gas shift reaction (Equation (3-9)), and reforming reaction (Equation (3-13)) results in more products and fewer reactants. When the steam to biomass mass ratio is greater than 0.1, the mole fraction of hydrogen decreases as more steam is introduced during gasification, leading to greater dilution of the reaction products. Consequently, this dilution causes a reduction in the mole fraction of hydrogen and carbon monoxide. From these findings, it can be inferred that the steam to biomass mass ratio between 0.1-0.2 is the appropriate range for hydrogen production.

From the study on hydrogen production through steam bagasse gasification, it is found that the gasification operated at gasifier temperature of 950 °C, gasifier pressure of 1 bar and steam to biomass mass ratio of 0.1 can provide the gas product, consisting of 50.82% H₂, 47.84% CO, 0.36% CO₂ and 0.30% CH₄. Thus, the purification process is required to obtain green hydrogen.

4.2.4 Effect of gasifier temperature and steam to biomass mass ratio on lower heating value

If the target of bagasse gasification is to produce syngas, it becomes crucial to take into account the lower heating value (LHV) as well. Figure 4.4 illustrates the influence of gasifier temperature on the lower heating value, while Figure 4.5 demonstrates the impact of the steam to biomass mass ratio on the lower heating value. Examining the lower heating value (LHV) of syngas described in Figure 4.4 reveals a direct correlation between the LHV and the operating temperature of the gasifier. The LHV of syngas increases as the gasifier operates at higher temperatures. This is attributed to the fact that LHV is derived from the mole fraction of carbon monoxide and hydrogen in syngas. As a result, it follows a similar trend to the profiles of carbon monoxide and hydrogen mole fractions. When the gasification reaction approaches completion at a temperature of 950°C, the LHV stabilizes at approximately 11.62 MJ/Nm³. Based on the simulation results, it can be concluded that the optimal operating temperature for the gasifier is 950°C.

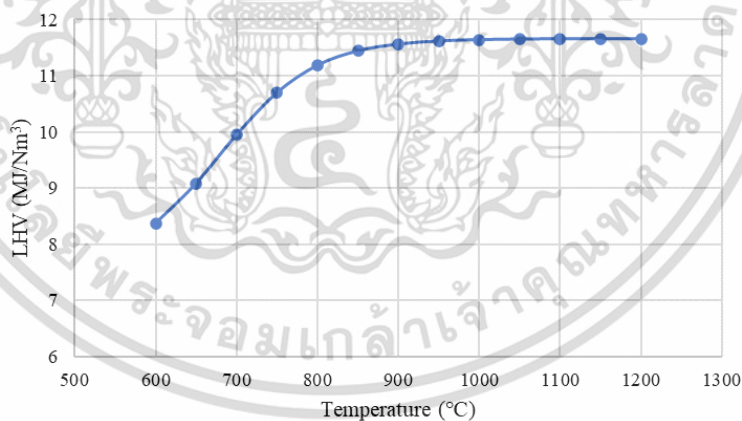


Figure 4.4 Effect of gasifier temperature on lower heating value at steam to biomass mass ratio of 0.1.

Furthermore, considering the LHV of syngas according to Figure 4.5, it becomes evident that the maximum LHV of 11.62 MJ/Nm³ is achieved at a steam to biomass mass ratio of 0.1. However, as the steam to biomass ratio increases beyond this point,

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the LHV of syngas decreases. This decline occurs due to the negative effects of excess steam in the system, impacting both the dilution of hydrogen with steam and the conversion of carbon monoxide to carbon dioxide. However, the main objective of this study was to concentrate on the production of hydrogen.

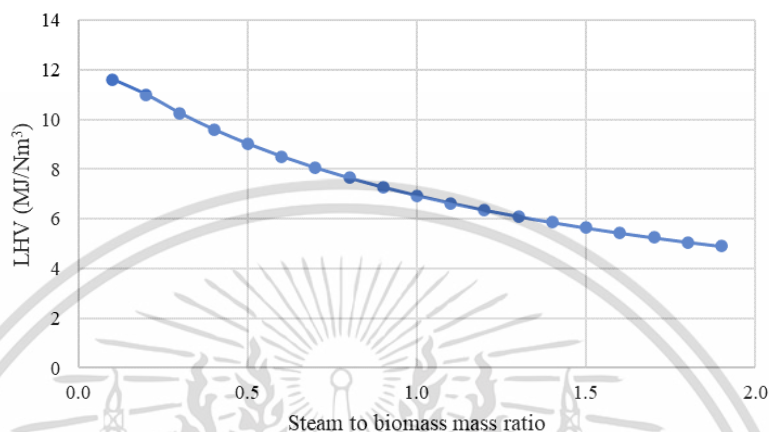


Figure 4.5 Effect of steam to biomass mass ratio on lower heating value at gasifier temperature of 950 °C.

4.3 Operating conditions in water gas shift process

This section presents the effects of operating conditions in water gas shift process including water gas shift reactor temperature and water to biomass mass ratio on hydrogen production.

4.3.1 Effect of water gas shift reactor temperature on hydrogen production

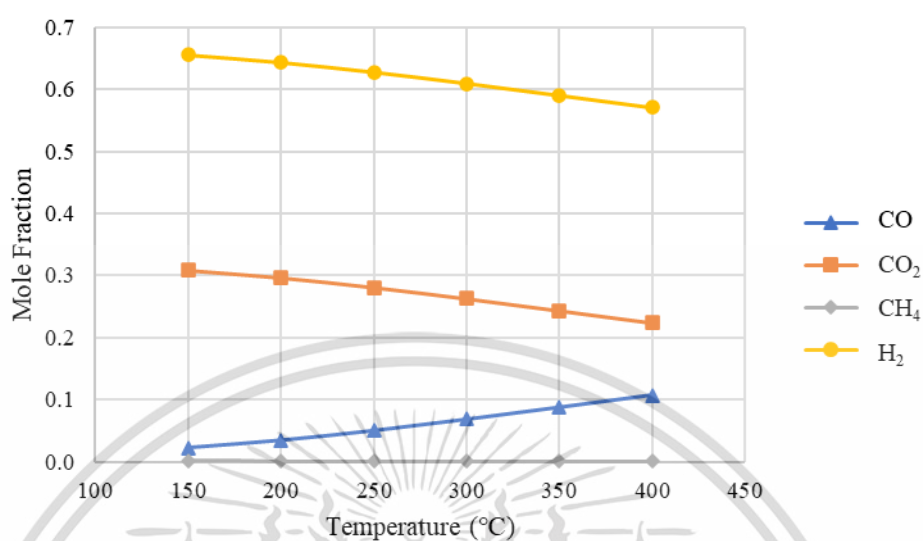


Figure 4.6 Effect of water gas shift reactor temperature on hydrogen production at water to biomass mass ratio of 0.6.

In the study, the effect of water gas shift reactor temperature on hydrogen production is demonstrated in Figure 4.6, with the water gas shift reactor temperature ranging from 150 to 400 °C while the water gas shift reactor pressure and water to biomass mass ratio are held constant at 1 bar and 0.6, respectively. The results indicate that increasing the water gas shift reactor temperature leads to an increase in the mole fraction of carbon monoxide while reducing the mole fraction of hydrogen and carbon dioxide and the mole fraction of methane is constant. This is because the high-temperature operation shifts the exothermic reaction of water gas shift reaction (Equation (3-9)) backward, resulting in higher carbon monoxide and lower hydrogen and carbon dioxide and methane is constant. As a result, the water gas shift reactor temperature of 150 °C is identified as the optimum due to its high mole fraction of hydrogen.

4.3.2 Effect of water to biomass mass ratio on hydrogen production

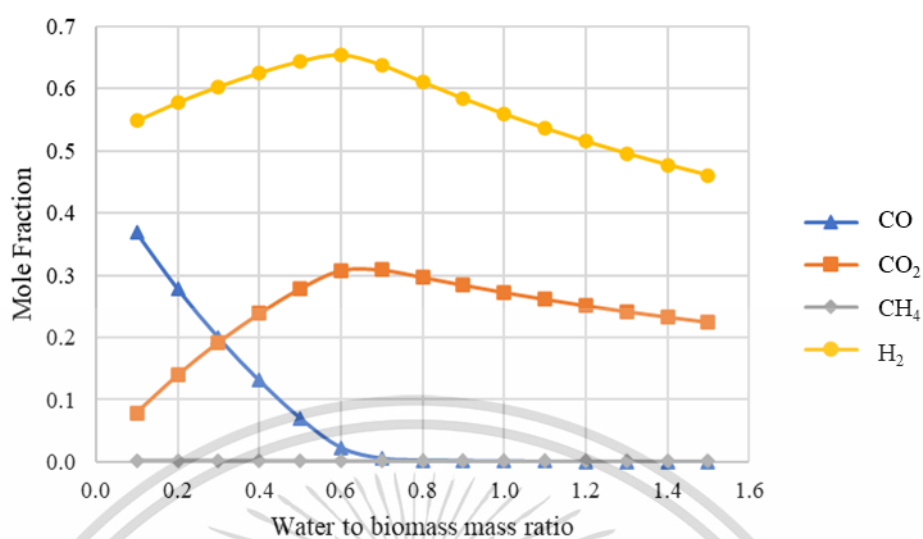


Figure 4.7 Effect of water to biomass mass ratio on hydrogen production at water gas shift reactor temperature of 150 °C.

In this study, the effect of water to biomass mass ratio on hydrogen production was analyzed and presented in Figure 4.7. The study focused on a range of ratios between 0.1 to 1.5, with the water gas shift reactor operating at temperature of 150°C and pressure of 1 bar. Increasing the water to biomass mass ratio leads to an increase in the mole fraction of hydrogen and carbon dioxide, while the mole fraction of carbon monoxide and methane decreases due to the addition of water to the water gas shift process. This causes a shift in the equilibrium of water gas shift reaction (Equation (3-9)), resulting in increased products and decreased reactants. The water gas shift reaction requires both carbon monoxide and water to proceed, and an excessive amount of water can reduce the concentration of carbon monoxide available for the reaction. This decrease in the mole fraction of carbon monoxide leads to a decrease in the mole fraction of hydrogen and carbon dioxide. In conclusion, it can be derived that a water to biomass mass ratio of 0.6 is the optimal ratio for highest hydrogen production.

Under the operation of water gas shift reactor at 150 °C, with water to biomass mass ratio of 0.6, the produced gas is composed of 65.50% H₂, 2.29% CO, 30.83% CO₂ and 0.20% CH₄. In order to provide the purified hydrogen, the carbon dioxide capture process is required as discussed in the next section.

4.4 Operating conditions in CaO adsorption

This section presents the influences of operating conditions in CaO adsorption including carbonator temperature, CaO to biomass mass ratio and regenerator temperature on hydrogen production.

4.4.1 Effect of carbonator temperature on hydrogen production

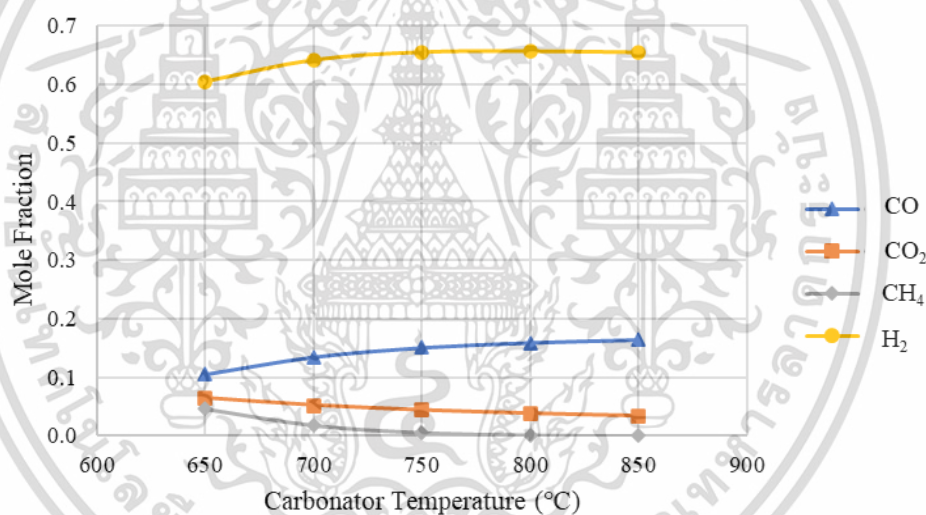


Figure 4.8 Effect of carbonator temperature on hydrogen production at a gasifier temperature of 950 °C, steam to biomass mass ratio of 0.1, CaO to biomass mass ratio of 1.9, and regenerator temperature of 900 °C.

In the study, the effect of carbonator temperature on hydrogen production is demonstrated in Figure 4.8, with the carbonator temperature ranging from 650 to 850 °C while the gasifier temperature, steam to biomass mass ratio, CaO to biomass mass ratio, and regenerator temperature are held constant at 950 °C, 0.1, 1.9 and 900,

respectively. The results indicate that increasing the carbonator temperature leads to an increase in the mole fraction of hydrogen and carbon monoxide while reducing the mole fraction of carbon dioxide and methane. The decrease in the mole fraction of carbon dioxide occurs due to the reaction between calcium oxide and carbon dioxide in the carbonator, resulting in the formation of calcium carbonate. Therefore, the mole fraction of carbon dioxide decreased, leading to an increase in the mole fractions of hydrogen and carbon monoxide. A lower amount of methane may be explained that the high-temperature operation may not only promotes carbonation reaction but also shifts reforming reaction (Equation (3-13)) forward, resulting in higher carbon monoxide and hydrogen and lower methane. From this study, the optimal carbonator temperature is 750 °C and this temperature is extremely high. This is because higher temperatures increase the rate of CO₂ adsorption onto the CaO surface. This results in faster and more efficient capture of CO₂ from the syngas, leading to higher CO₂ removal efficiency during the adsorption process.

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4.4.2 Effect of CaO to biomass mass ratio on hydrogen production

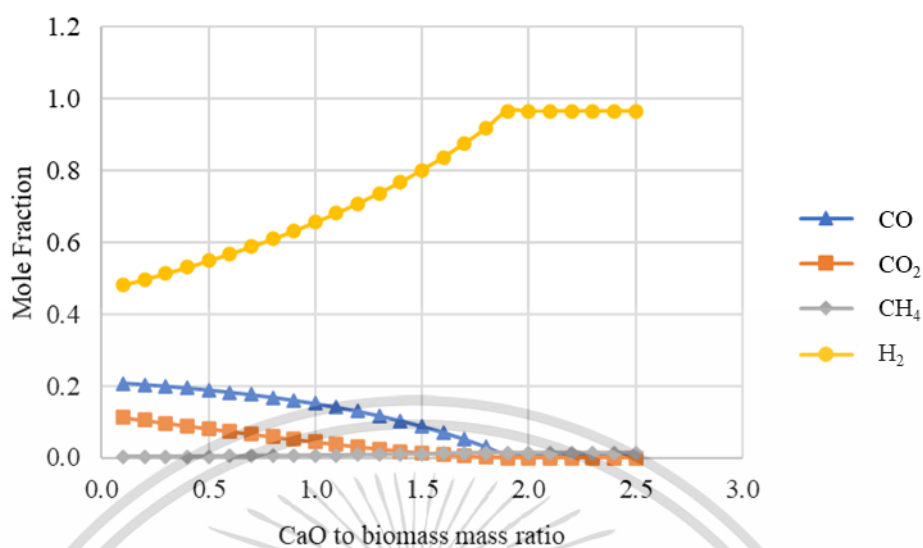


Figure 4.9 Effect of CaO to biomass mass ratio on hydrogen production at a gasifier temperature of 950 °C, steam to biomass mass ratio of 0.1, carbonator temperature of 750 °C and regenerator temperature of 900 °C.

In this study, the effect of CaO to biomass mass ratio on hydrogen production is analyzed and presented in Figure 4.9. This study focuses on a range of ratios between 0.1 to 2.5, with the gasifier temperature of 950 °C, steam to biomass mass ratio of 0.1, carbonator temperature of 750 °C and regenerator temperature of 900 °C. Increasing the CaO to biomass mass ratio leads to a significant increase in the mole fraction of hydrogen, while the mole fraction of carbon monoxide, carbon dioxide and methane decreases. This can be explained by the capture of carbon dioxide by CaO, which influences the water gas shift reaction (Equation (3-9)). As a result, the reduction in the mole fraction of carbon dioxide due to CaO adsorption stimulates a rapid forward shift of carbon monoxide and water in the water gas shift reaction, resulting in an increased mole fraction of hydrogen and a decreased mole fraction of carbon monoxide. In conclusion, it can be derived that a CaO to biomass mass ratio of 1.9 is the optimal ratio for hydrogen production.

4.4.3 Effect of regenerator temperature on CO₂ removal

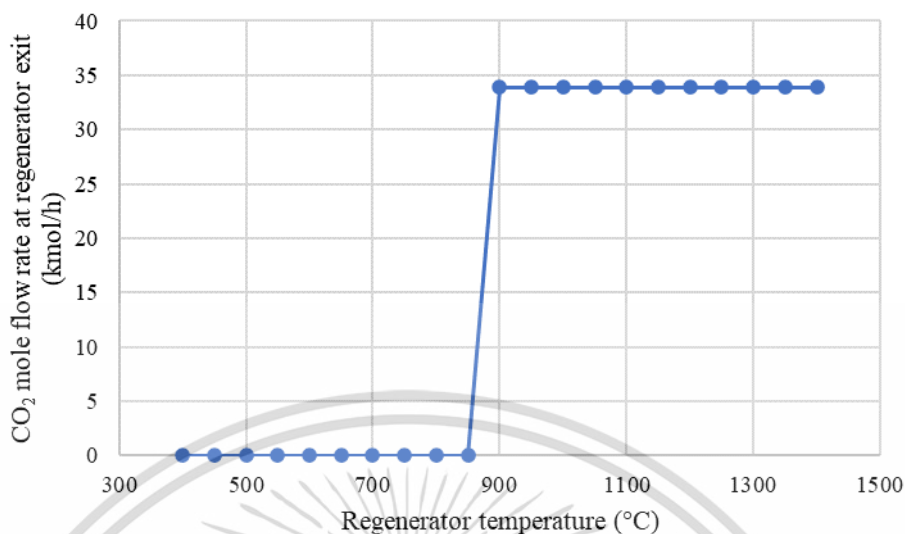


Figure 4.10 Effect of regenerator temperature on the CO₂ mole flow rate released from CaCO₃ at a gasifier temperature of 950 °C, steam to biomass mass ratio of 0.1, CaO to biomass mass ratio of 1.9, and carbonator temperature 750 °C.

Based on the data presented in Figure 4.10, the effect of the regenerator temperature within the range of 400 °C and 1400 °C on levels of carbon dioxide is studied. This study focuses on molar flow rate of carbon dioxide exited from a regenerator since the regenerator is responsible for releasing the adsorbed CO₂ from the CaO sorbent, regenerating the sorbent material for reuse. The molar flow rate of CO₂ exiting the regenerator indicates how effectively the adsorbed CO₂ is being released from the sorbent. A high molar flow rate of CO₂ suggests efficient desorption and regeneration, leading to better CO₂ capture efficiency. The simulation data shows that carbon dioxide desorption from the regenerator initiates around 850 - 900 °C. However, when the temperature exceeds 900 °C, the concentration of carbon dioxide remains constant. Based on this study, it can be concluded that the optimal regenerator temperature for the CaO adsorption process is 900 °C.

From the investigation on CaO adsorption, it is found that the carbonator and generator should be operated at 750 °C and 900 °C, with CaO to biomass mass ratio

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of 1.9. Under these operating conditions, the gas product, composed of 96.53% H₂, 0.86% CO, 0.01% CO₂ and 1.3% CH₄ can be provided. The integration of steam bagasse gasification, water gas shift reactor, and CaO adsorption enables the production of green hydrogen with a high purity level of 99.95%.

4.5 Summary of green hydrogen production through steam gasification from bagasse integrated with CaO adsorption

From the simulation results of steam gasification integrated with CaO adsorption reported in Sections 4.2-4.4, it can be concluded the optimal operating conditions of gasification, water gas shift reactor and CaO adsorption as Tables 4.2. The gas composition obtained from this process is summarized in Table 4.3 Table 4.4 shows the data of each stream in a flowsheet, while Table 4.5 lists the heat duty of each unit used in steam gasification integrated with CaO adsorption under the optimal operating condition. When the energy analysis is determined, it is found that the overall energy efficiency is 41.42%.

Table 4.2 Optimal operating conditions of gasification, water gas shift reactor and CaO adsorption

Parameter	Operating conditions
Gasification	
Gasifier temperature (°C)	950
Gasifier pressure (bar)	1
Steam to biomass mass ratio	0.1
Water gas shift reactor	
Water gas shift reactor temperature (°C)	150
Water to biomass mass ratio	0.6

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Table 4.2 Optimal operating conditions of gasification, water gas shift reactor and CaO adsorption (Cont.)

Parameter	Operating conditions
CaO adsorption	
Carbonator temperature (°C)	750
CaO to biomass mass ratio	1.9
Regenerator temperature (°C)	900

Table 4.3 The gas composition obtained from the steam gasification from bagasse integrated with CaO adsorption

Gas composition	Mole Fraction	Mole Flow rate (kmol/hr)
H ₂	0.9995	68.5658
H ₂ O	0.0004	0.0332
H ₂ purity (%)		99.95
Efficiency of CO ₂ capture (%)		99.96

Table 4.4 Data of each stream in a flowsheet of green hydrogen production through steam gasification from bagasse integrated with CaO adsorption

Stream	Temperature (°C)	Pressure (bar)
Gasification		
BAGASSE	25	1
STEAM1	25	1
STEAM2	150	1
INGASIF	950	1
OUTGASIF	950	1

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Table 4.4 Data of each stream in a flowsheet of green hydrogen production through steam gasification from bagasse integrated with CaO adsorption (Cont.)

Stream	Temperature (°C)	Pressure (bar)
Gasification		
ASH	950	1
INWGS	950	1
Water gas shift reactor		
INWGS	950	1
WATER	25	1
STEAM3	150	1
LIQ	150	1
INADSORB	150	1
CaO adsorption		
INADSORB	150	1
CAO	25	1
CAO-2	700	1
OUTADSORB	750	1
CACO3	750	1
OUTDESORB	900	1
CO2	900	1
RE-CAO	900	1
LEAN-CO2	750	1
GAS	750	1
H2	750	1
H2++	25	1
CONDENSA	20	50
HYDROGEN	20	50

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Table 4.5 Heat duty of each unit used in steam gasification integrated with CaO adsorption under the optimal operating condition

Stream	Heat duty (kW)
Gasification	
DECOMP	2066.38
HEATER1	76.99
GASIF	-382.24
SEP-ASH	0.00
Water gas shift reactor	
WGS	-870.29
HEATER2	461.941
CaO adsorption	
ADSORBER	-1025.44
HEATER3	326.09
SEP-1	0.00
DESORBER	1784.34
DESORBER	1784.34
SEP-2	0.00
SEP-GAS	0.00
COOLER1	-413.23
FLASH	-13.00

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CHAPTER V

SUPERCRITICAL WATER BAGASSE GASIFICATION

This chapter focuses on the supercritical water gasification of bagasse integrated with CaO adsorption to produce the green hydrogen. Section 5.1 presents the comparison of results of gas product between the simulation results and experimental data extracted from the literature of supercritical water gasification of biomass. Section 5.2 presents the impact of operating conditions in supercritical water gasification on hydrogen production and lower heating value. Section 5.3 presents the effects of operating conditions in water gas shift process while Section 5.4 describes the effect of CaO adsorption operating conditions on hydrogen production. Finally, the summary of this study is described in Section 5.5.

5.1 Comparison results between simulation and experiment

In this section, the experiment of Wang et al.⁵ is used to compare with the simulation result. Wang et al.⁵ performed supercritical water gasification on wheat straw in which the ultimate and proximate analysis data provided in Table 3.3. In their experiment, the gasifier operated at a pressure of 230 bar and temperature of 750 °C, using a supercritical water to biomass mass ratio of 1. Table 5.1 presents the comparison results for supercritical water gasification obtained from both experiment and simulation. It can be seen that under the same feedstock and same operating condition with the experiment, the simulation results show similar trends to the experimental data. The mean absolute error (MAE) is 0.025, which does not exceed 10 and is an acceptable value.

Table 5.1 The comparison of syngas production from wheat straw between experimental results by Wang et al.⁵ and simulation results in this study.

Syngas composition (Mole Fraction)	Experiment	Simulation
CO	0.07	0.07
CO ₂	0.40	0.35
CH ₄	0.31	0.33
H ₂	0.23	0.26
MAE	0.025	

5.2 Operating conditions in supercritical water gasification

This section presents the effects of operating conditions in gasification including gasifier temperature, gasifier temperature and supercritical water to biomass mass ratio on hydrogen production.

5.2.1 Effect of gasifier temperature on hydrogen production

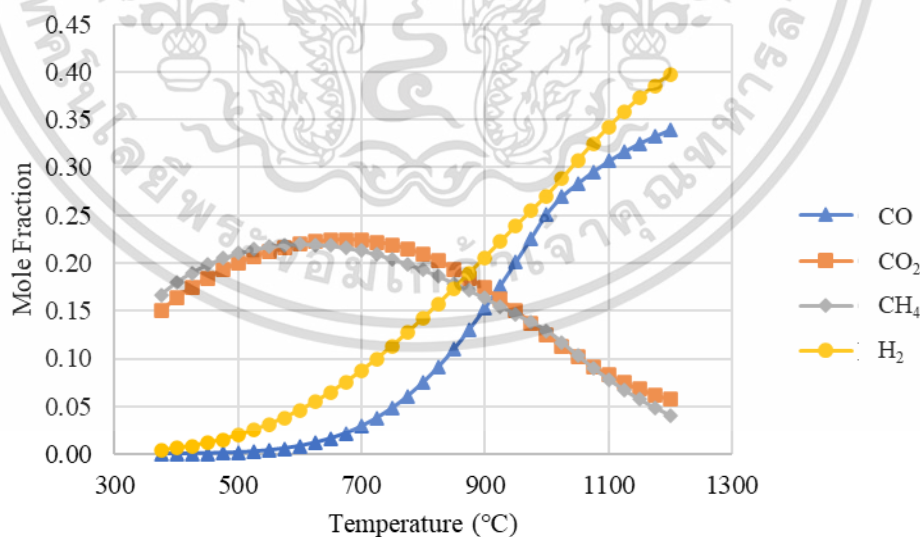


Figure 5.1 Effect of gasifier temperature on hydrogen production at gasifier pressure of 221 bar and supercritical water to biomass mass ratio of 0.4.

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In the study, the effect of gasifier temperature on hydrogen production is demonstrated in Figure 5.1, with the gasifier temperature ranging from 600 to 1200 °C while the gasifier pressure and supercritical water to biomass mass ratio are held constant at 221 bar and 0.4, respectively. The results indicate that increasing the gasifier temperature leads to an increase in the mole fraction of carbon monoxide and hydrogen while reducing the mole fraction of carbon dioxide and methane. This is because the high-temperature operation promotes the endothermic reactions that include Boudouard reaction (Equation (3-6)), water-gas reaction (Equation (3-7)), and reforming reaction (Equation (3-13)) to the product side. This causes higher carbon monoxide and hydrogen and lower carbon dioxide and methane. As a result, the optimum gasifier temperature is 1200 °C due to its high mole fraction of hydrogen.

5.2.2 Effect of gasifier pressure on hydrogen production

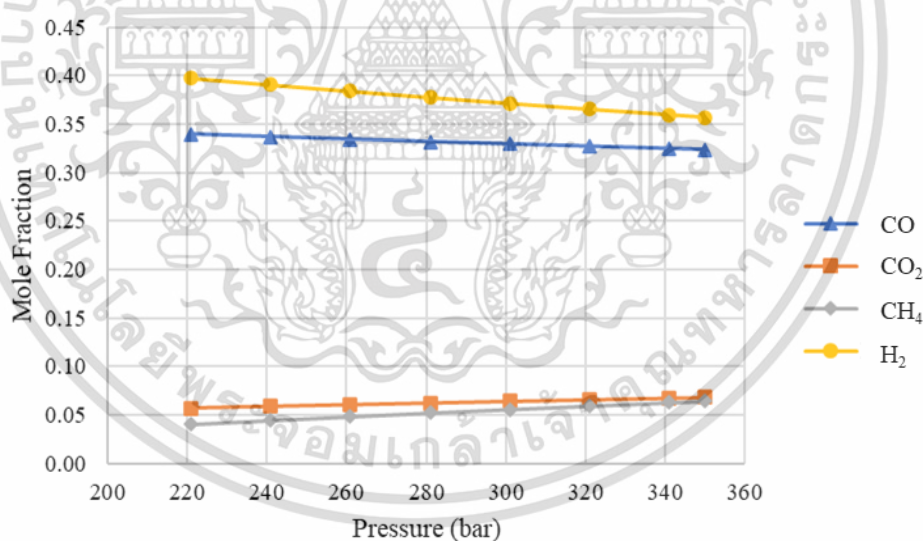


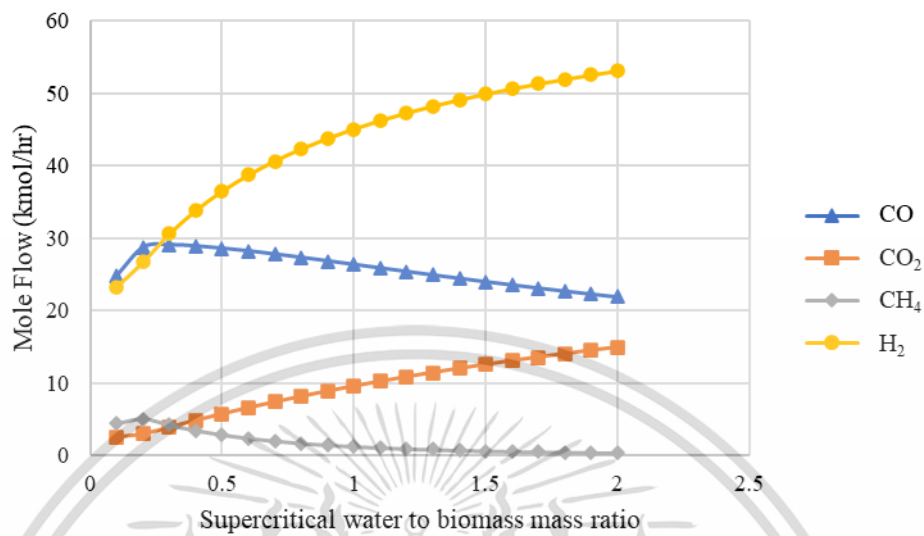
Figure 5.2 Effect of gasifier pressure on hydrogen production at gasifier temperature of 1200 °C and supercritical water to biomass mass ratio of 0.4.

This study presents the effect of gasifier pressure on hydrogen production, as illustrated in Figure 5.2, where the gasifier pressure is varied from 221 to 350 bar while

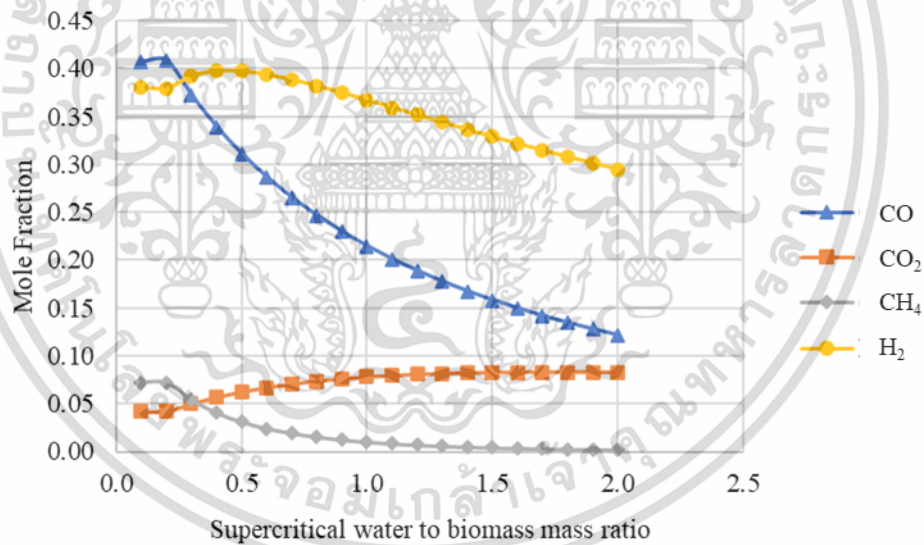
maintaining a fixed gasifier temperature and supercritical water to biomass mass ratio at 1200 °C and 0.4, respectively. The simulation results show that as gasifier pressure increases, the mole fraction of carbon dioxide and methane also increases, while the mole fraction of carbon monoxide and hydrogen decreases. This can be explained by Le Châtelier's principle, which explains that increasing pressure can shift the chemical equilibrium towards the side with fewer gaseous moles, whereas decreasing pressure can shift the equilibrium towards the side with more gaseous moles. After analyzing the chemical reactions involved in gasification, specifically Equations (3-1), (3-8), (3-10), (3-11), (3-12), and (3-13), it was discovered that the number of moles on the reactant side is greater than that on the product side, indicating that the reaction will proceed forward. Based on the simulation results, it is recommended to maintain the gasifier pressure of 221 bar to maintain a high mole fraction of hydrogen.

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5.2.3 Effect of supercritical water to biomass mass ratio on hydrogen production



(a) Molar flow rate of gas product



(b) Mole fraction of gas product

Figure 5.3 Effect of supercritical water to biomass mass ratio on (a) molar flow rate of gas product and (b) mole fraction of gas product at gasifier temperature of 1200 °C, gasifier pressure of 221 bar

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In this study, the effect of supercritical water to biomass mass ratio on hydrogen production is examined, as illustrated in Figure 5.3. The supercritical water to biomass mass ratio is varied in a range of 0.1 to 2.0, with the gasifier operating at temperature of 1200°C and pressure of 221 bar. Figure 5.3(a) shows the effect of steam to biomass mass ratio on molar flow rate of gas product. The results reveal that when there is more steam relative to biomass, the production of hydrogen increases. The rationale remains consistent in Section 4.2.3.

Figure 5.3(b) demonstrates that increasing the supercritical water to biomass mass ratio, within the range of 0.1 to 0.4, results in higher mole fractions of hydrogen and carbon dioxide, while the mole fractions of carbon monoxide and methane decrease. The addition of supercritical water to the gasification process causes a shift in the equilibrium of water gas reaction (Equation (3-7)), water gas shift reaction (Equation (3-9)), and reforming reaction (Equation (3-13)), leading to increased product formation and reduced reactants. However, when the supercritical water to biomass mass ratio exceeds 0.4, the simulation indicates a decline in the mole fraction of hydrogen. This is because an increased amount of supercritical water in the gasification process causes higher dilution of the reaction products, leading to a decrease in the mole fraction of hydrogen and carbon monoxide. Therefore, it can be inferred that a supercritical water to biomass mass ratio of 0.4 represents the appropriate range for hydrogen production.

From the study on hydrogen production through supercritical water bagasse gasification, it is found that the gasification operated at gasifier temperature of 1200 °C, gasifier pressure of 221 bar and supercritical water to biomass mass ratio of 0.4, can provide the gas product, consisting of 39.75% H₂, 33.95% CO, 5.71% CO₂ and 4.04%CH₄. Thus, the purification process is required to obtain green hydrogen.

5.2.4 Effect of gasifier temperature and supercritical water to biomass mass ratio on lower heating value

If the target of bagasse gasification is to produce syngas, it becomes crucial to take into account the lower heating value (LHV) as well. Figure 5.4 illustrates the influence of gasifier temperature on the lower heating value, while Figure 5.5 demonstrates the impact of the supercritical water to biomass mass ratio to biomass mass ratio on the lower heating value. From Figure 5.4, it is found that The LHV of syngas increases as the gasifier operates at higher temperatures. This is attributed to the fact that LHV is derived from the mole fraction of carbon monoxide and hydrogen in syngas. As a result, it follows a similar trend to the profiles of carbon monoxide and hydrogen mole fractions. When the gasification reaction approaches a temperature of 1000°C, the LHV maximizes at approximately 10.73 MJ/Nm³. Based on the simulation results, it can be concluded that the optimal operating temperature for the gasifier is 1000°C.

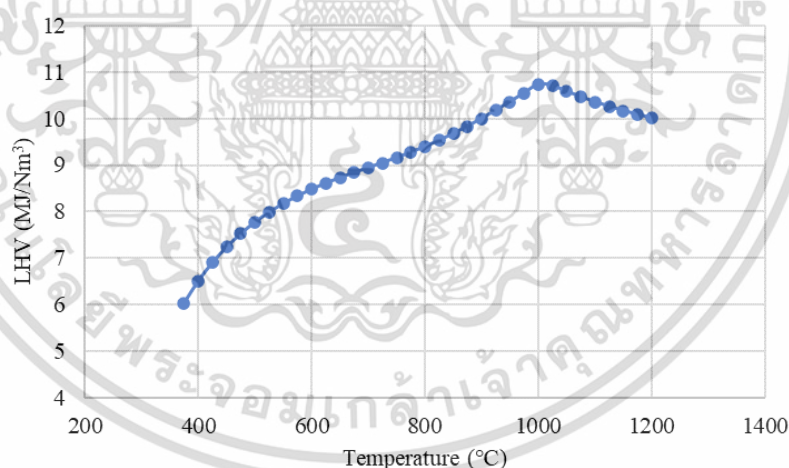


Figure 5.4 Effect of gasifier temperature on lower heating value at supercritical water to biomass mass ratio of 0.4.

Furthermore, considering the LHV of syngas according to Figure 5.5, it becomes evident that the maximum LHV of 11.83 MJ/Nm³ is achieved at a supercritical to biomass mass ratio of 0.1. However, as the supercritical water to biomass ratio

increases beyond this point, the LHV of syngas decreases. This decline occurs due to the negative effects of excess supercritical water in the system, impacting both the dilution of hydrogen with supercritical water and the conversion of carbon monoxide to carbon dioxide. However, the main objective of this study was to concentrate on the production of hydrogen.

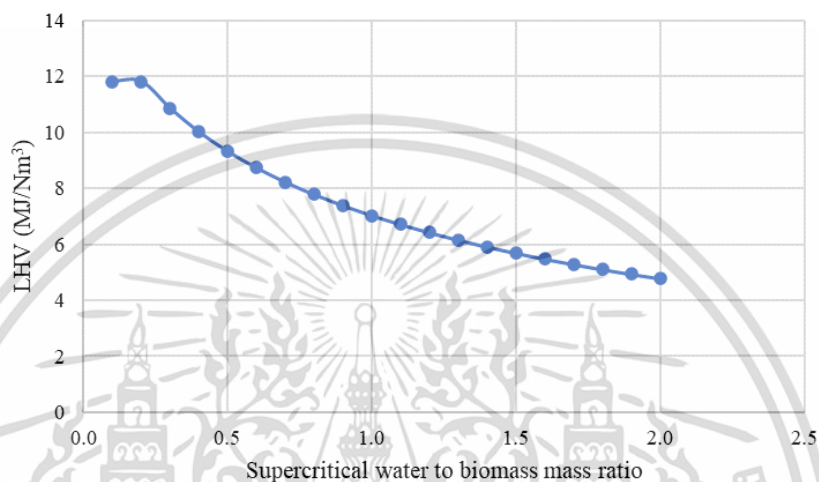


Figure 5.5 Effect of supercritical water to biomass mass ratio on lower heating value at gasifier temperature of 1200 °C.

5.3 Operating conditions in water gas shift process

This section presents the effects of operating conditions in water gas shift process including water gas shift reactor temperature and water to biomass mass ratio on hydrogen production.

5.3.1 Effect of water gas shift reactor temperature on hydrogen production

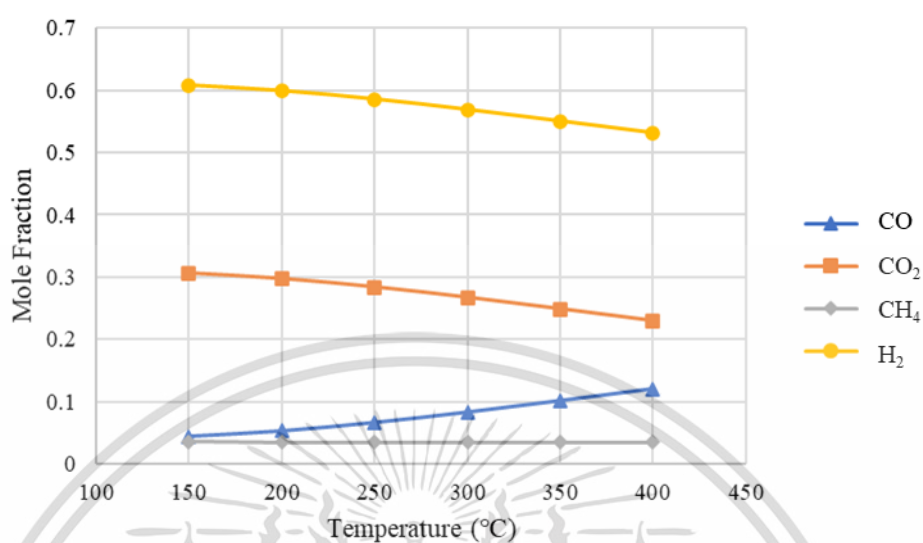


Figure 5.6 Effect of water gas shift reactor temperature on hydrogen production at water to biomass mass ratio of 0.2.

In the study, the effect of water gas shift reactor temperature, varying between 150 and 400 °C, on hydrogen production is demonstrated in Figure 5.6 while the water gas shift reactor pressure and water to biomass mass ratio are held constant at 1 bar and 0.2, respectively. The results indicate that increasing the water gas shift reactor temperature causes an increase in the mole fraction of carbon monoxide while reducing the mole fraction of hydrogen and carbon dioxide and the mole fraction of methane is constant. This is because the high-temperature operation promotes the water gas shift reaction (Equation (3-9)) as exothermic reaction being shifted backward, resulting in higher carbon monoxide and lower hydrogen and carbon dioxide and methane is constant. As a result, the temperature of water gas shift reactor at 150 °C is identified as the optimum due to its high mole fraction of hydrogen.

5.3.2 Effect of water to biomass mass ratio on hydrogen production

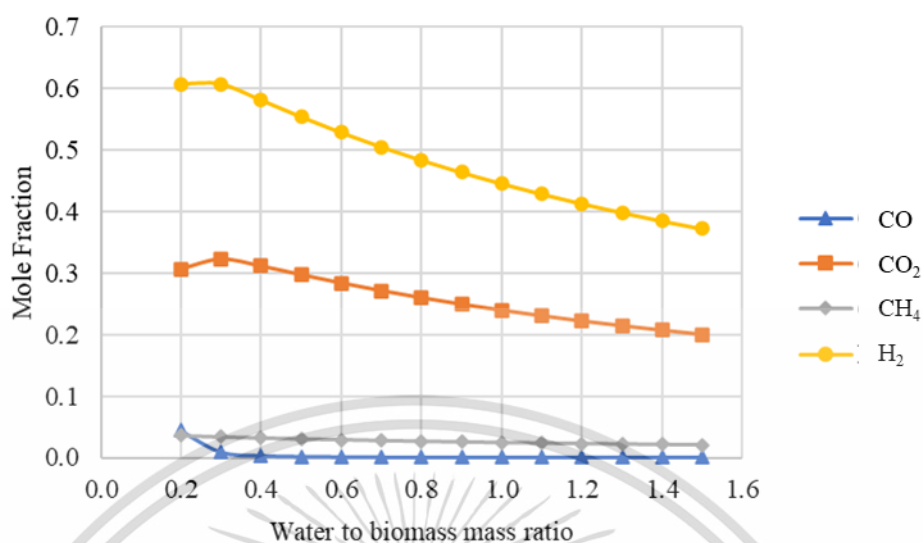


Figure 5.7 Effect of water to biomass mass ratio on hydrogen production at water gas shift reactor temperature of 150 °C.

Figure 5.7 presents the effect of water to biomass mass ratio on hydrogen production. The study focuses on a range of water to biomass mass ratio between 0.2 to 1.5, with the water gas shift reactor operating at temperature of 150°C and pressure of 1 bar. Increasing the water to biomass mass ratio leads to an increase in the mole fraction of hydrogen and carbon dioxide, while the mole fraction of carbon monoxide and methane decreases. The water gas shift reaction (Equation (3-9)) requires both carbon monoxide and water to proceed, and an excessive amount of water can reduce the concentration of carbon monoxide available for the reaction. This decrease in the mole fraction of carbon monoxide leads to a decrease in the mole fraction of hydrogen and carbon dioxide. In conclusion, it can be derived that a water to biomass mass ratio of 0.2 is the optimal ratio for highest hydrogen production.

Under the operation of water gas shift reactor at 150 °C, with water to biomass mass ratio of 0.2, the produced gas is composed of 60.75% H₂, 4.45% CO, 30.63% CO₂

and 3.57% CH₄. In order to provide the purified hydrogen, the carbon dioxide capture process is required as discussed in the next section.

5.4 Operating conditions in CaO adsorption

This section presents the effects of operating conditions in CaO adsorption including carbonator temperature, calcium oxide to biomass mass ratio and regenerator temperature on hydrogen production.

5.4.1 Effect of carbonator temperature on hydrogen production

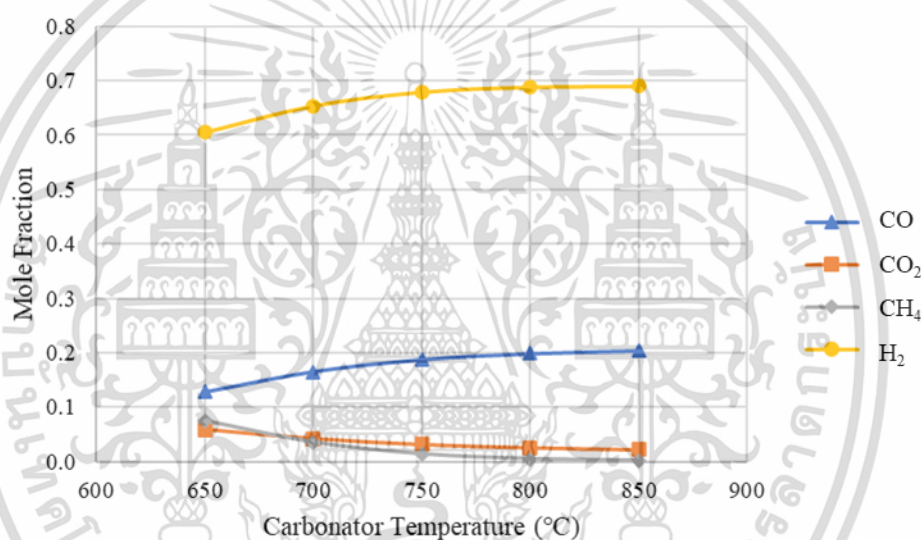


Figure 5.8 Effect of carbonator temperature on the mole fraction of gas product composition exited from a carbonator at a gasifier temperature of 1200°C, supercritical water to biomass mass ratio of 0.4, CaO to biomass mass ratio of 1.78, and regenerator temperature 900 °C.

The effect of carbonator temperature, which is adjusted in a range of 650 to 850 °C, on hydrogen production is demonstrated in Figure 5.8 while the gasifier temperature, supercritical water to biomass mass ratio, CaO to biomass mass ratio, and regenerator temperature are held constant at 1200 °C, 0.4, 1.78 and 900 °C, respectively. The results indicate that increasing the carbonator temperature results

in an increase in the mole fraction of hydrogen and carbon monoxide while reducing the mole fraction of carbon dioxide and methane. This is because the high-temperature operation promotes the endothermic reactions being shifted forward such as reforming reaction (Equation (3-13)) resulting in higher carbon monoxide and hydrogen and lower methane. The decrease in the mole fraction of carbon dioxide occurs due to the reaction between calcium oxide and carbon dioxide in the carbonator, resulting in the formation of calcium carbonate. Therefore, the mole fraction of carbon dioxide can be decreased, leading to an increase in the mole fractions of hydrogen and carbon monoxide. From this study, the optimal carbonator temperature is 800 °C. The rationale behind utilizing high temperatures remains consistent with the explanation provided in Section 4.4.1.

5.4.2 Effect of CaO to biomass mass ratio on hydrogen production

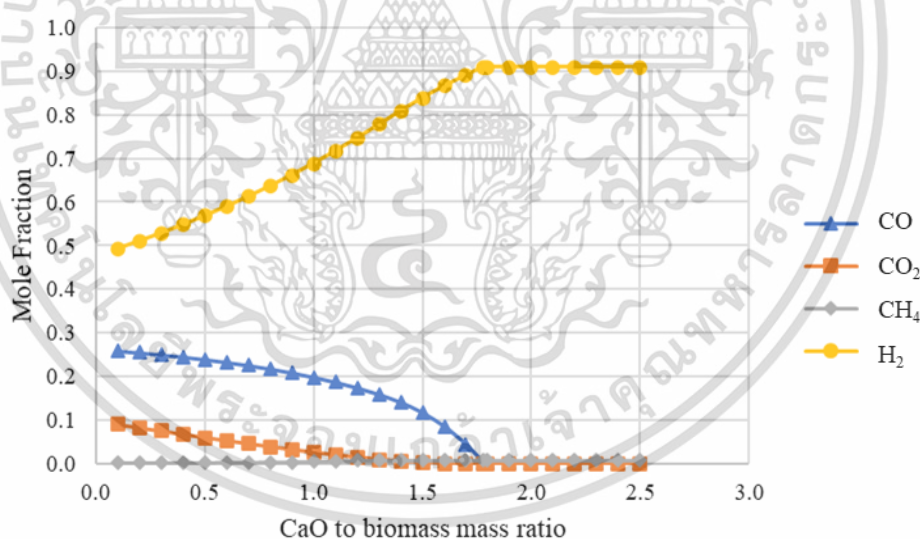


Figure 5.9 Effect of calcium oxide to biomass mass ratio on hydrogen production at a gasifier temperature of 1200 °C, supercritical water to biomass mass ratio of 0.4, carbonator temperature of 800 °C and regenerator temperature 900 °C.

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This section presents the effect of CaO to biomass mass ratio on hydrogen, shown in Figure 5.9. The CaO to biomass mass ratio is changed between 0.1 to 2.5 while the gasifier temperature of 1200 °C, supercritical water to biomass mass ratio of 0.4, carbonator temperature of 800 °C and regenerator temperature of 900 °C are specified. Increasing the CaO to biomass mass ratio leads to a significant increase in the mole fraction of hydrogen, while the mole fraction of carbon monoxide, carbon dioxide and methane decreases. This can be explained by the capture of carbon dioxide by CaO, which influences the water gas shift reaction (Equation (3-9)). As a result, the reduction in the mole fraction of carbon dioxide due to CaO adsorption stimulates a rapid forward shift of carbon monoxide and water in the water gas shift reaction, resulting in an increased mole fraction of hydrogen and a decreased mole fraction of carbon monoxide. In conclusion, it can be derived that a calcium oxide to biomass mass ratio of 1.78 is the optimal ratio for hydrogen production.

5.4.3 Effect of regenerator temperature on CO₂ removal

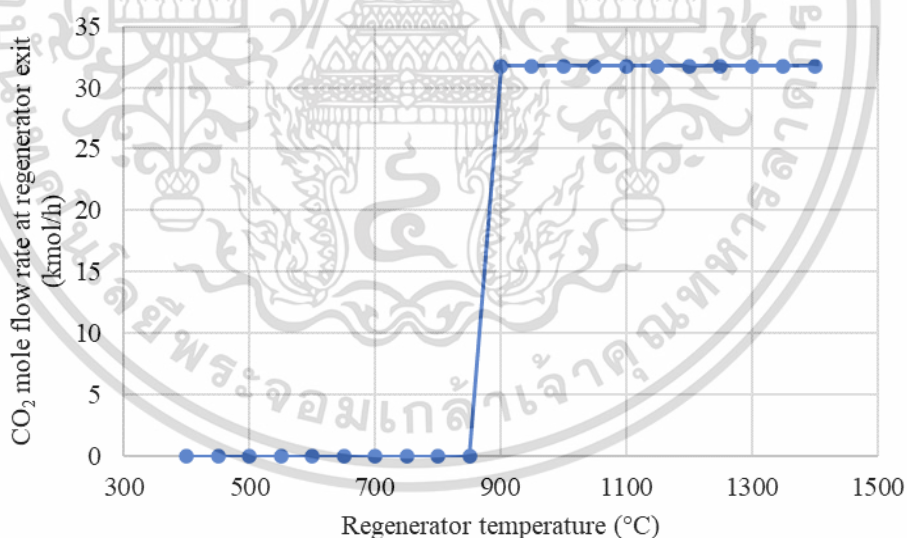


Figure 5.10 Effect of regenerator temperature on the CO₂ mole flow rate released from CaCO₃ at a gasifier temperature of 1200 °C, supercritical water to biomass mass ratio of 0.4, CaO to biomass mass ratio of 1.78, and carbonator temperature 800 °C.

Figure 5.10 illustrates the effect of the regenerator temperature within the range of 400 °C and 1400 °C on levels of carbon dioxide, while maintaining the gasifier temperature of 1200 °C, supercritical water to biomass mass ratio of 0.4, calcium oxide to biomass mass ratio of 1.78, and carbonator temperature 800 °C. The simulation results show that carbon dioxide desorption from the regenerator initiates around 850 - 900 °C. However, when the temperature exceeds 900 °C, the concentration of carbon dioxide remains constant. Based on this study, it can be concluded that the optimal regenerator temperature for the calcium oxide adsorption process is 900 °C.

From the investigation on CaO adsorption, it is found that the carbonator and generator should be operated at 800 °C and 900 °C, with CaO to biomass mass ratio of 1.78. Under these operating conditions, the gas product, composed of 90.97% H₂, 0.28% CO, 0.00% CO₂ and 8.6% CH₄ can be provided. The integration of supercritical water bagasse gasification, water gas shift reactor, and CaO adsorption enables the production of green hydrogen with a high purity level of 99.98%.

5.5 Summary of green hydrogen production through supercritical water gasification from bagasse integrated with CaO adsorption

From the simulation results of supercritical water gasification integrated with CaO adsorption reported in Sections 5.2-4.4, it can be concluded the optimal operating conditions of gasification, water gas shift reactor and CaO adsorption as Tables 5.2. The gas composition obtained from this process is summarized in Table 5.3 Table 5.4 shows the data of each stream in a flowsheet, while Table 5.5 lists the heat duty of each unit used in steam gasification integrated with CaO adsorption under the optimal operating condition. When the energy analysis is determined, it is found that the overall energy efficiency is 26.01%.

Table 5.2 Optimal operating conditions of gasification, water gas shift reactor and CaO adsorption

Parameter	Operating conditions
Gasification	
Gasifier temperature (°C)	1200
Gasifier pressure (bar)	221
Supercritical water to biomass mass ratio	0.4
Water gas shift	
Water gas shift reactor temperature (°C)	150
Water to biomass mass ratio	0.2
CaO adsorption	
Carbonator temperature (°C)	800
CaO to biomass mass ratio	1.78
Regenerator temperature (°C)	900

Table 5.3 The gas composition obtained from the supercritical water gasification from bagasse integrated with CaO adsorption

Gas composition	Mole Fraction	Mole Flow rate (kmol/hr)
H ₂	0.9998	55.2620
H ₂ O	0.0002	0.0087
H ₂ purity (%)	99.98	
Efficiency of CO ₂ capture (%)	99.99	

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Table 5.4 Data of each stream in a flowsheet of green hydrogen production through supercritical water gasification from bagasse integrated with CaO adsorption

Stream	Temperature (°C)	Pressure (bar)
Gasification		
BAGASSE	25	1
STEAM1	25	1
STEAM2	39	221
SCW	375	221
INGASIF	1200	221
OUTGASIF	1200	221
ASH	1200	221
INWGS	1200	221
Water gas shift reactor		
INWGS	1200	221
WATER	25	1
STEAM3	150	1
LIQ	150	1
INADSORB	150	1
CaO adsorption		
INADSORB	150	1
CAO	25	1
CAO-2	800	1
OUTADSOR	800	1
CACO3	800	1
OUTDESOR	900	1
CO2	900	1

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Table 5.4 Data of each stream in a flowsheet of green hydrogen production through supercritical water gasification from bagasse integrated with CaO adsorption (Cont.)

Stream	Temperature (°C)	Pressure (bar)
CaO adsorption (Cont.)		
RE-CAO	900	1
LEAN-CO2	800	1
GAS	800	1
H2	800	1
HYDROGEN	25	1

Table 5.5 Heat duty of each unit used in steam gasification integrated with CaO adsorption under the optimal operating condition

Stream	Heat duty (kW)
Gasification	
DECOMP	2288.5
PUMP	9.74
HEATER1	264.56
GASIF	-371.756
SEP-ASH	0.00
Water gas shift reactor	
WGS	-1167.28
HEATER2	153.98
CaO adsorption	
ADSORBER	-1012.89
HEATER3	352.76
SEP-1	0.00

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Table 5.5 Heat duty of each unit used in steam gasification integrated with CaO adsorption under the optimal operating condition (Cont.)

Stream	Heat duty (kW)
CaO adsorption (Cont.)	
DESORBER	1617.11
SEP-2	0.00
SEP-GAS	0.00
COOLER1	-351.48



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CHAPTER VI

CONCLUSION

6.1 Conclusions

In this research, green hydrogen production from bagasse gasification integrated with CaO adsorption was designed and simulated through the Aspen Plus version 12 simulation software program. Thermodynamic calculations were performed using the Peng-Robinson equation of state with Boston-Mathias modifications. The equilibrium gas compositions during biomass gasification were obtained using the minimum Gibbs free energy method. Steam and supercritical water were employed as gasifying agents in the biomass gasification process. The proposed model was employed to identify the optimal operating conditions for green hydrogen production through bagasse gasification integrated with CaO adsorption.

Firstly, the key parameters for steam bagasse gasification included gasifier temperature, gasifier pressure, and steam to biomass mass ratio were determined. In general, raising the temperature of the gasifier leads to an increase in hydrogen generation. The pressure in the gasifier primarily impacts the thermodynamics of the gasification process, with higher pressures not being favorable for hydrogen production. The steam to biomass ratio plays a crucial role in gasification. Increasing the steam to biomass ratio generally enhances hydrogen production. A higher steam helps to control the gasification reactions, particularly the water-gas shift reaction, which increases the production of hydrogen. However, it is important to note that there is an optimal range for the steam to biomass ratio, and exceeding this range can lead to excessive dilution and reduced hydrogen production. From the simulation results, it was found that the steam gasification of bagasse should be conducted at temperature of 950 °C, pressure of 1 bar, and steam to biomass mass ratio of 0.1 to

achieve maximum hydrogen production with a purity of 50.82%. However, since this

เอกสารนี้เป็นเอกสารที่สงวนลิขสิทธิ์สำหรับการใช้งานเพื่อการศึกษาเท่านั้น เมื่ออนุญาตให้เผยแพร่ไปใช้ประโยชน์ด้านการค้า
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process also contains high amounts of carbon monoxide, the installation of a water gas shift process is necessary to effectively remove carbon monoxide. Then, the effect of operating conditions in water gas shift reactor were examined. The simulation results indicated that maximum hydrogen production with a purity of 65.50% can be achieved when the water gas shift reactor operated at temperature of 150 °C and water to biomass mass ratio of 0.6. Finally, to achieve green hydrogen production, CaO adsorption was employed for CO₂ capture. The simulation indicated that CaO adsorption should be conducted at carbonator temperature of 750 °C, CaO to biomass mass ratio of 1.9, and regenerator temperature of 900 °C. The integration of bagasse steam gasification with CaO adsorption resulted in the production of green hydrogen with a purity of 99.95% and molar flow rate of 68.57 kmol/hr. Under the optimal operating conditions of all units, the energy efficiency is 41.42%.

Similar to steam bagasse gasification, it was found that the supercritical water gasification of bagasse should be carried out at temperature of 1200 °C, pressure of 221 bar, and supercritical water to biomass mass ratio of 0.4. Under these operating conditions, hydrogen production with a purity of 39.75% can be provided. Considering the installation of a water gas shift process, the simulation results showed that water gas shift reactor operating at 150 °C with water to biomass mass ratio of 0.2 can obtain the maximum hydrogen production with a purity of 60.75%. It can be observed that the gas product obtained from supercritical water gasification contains high amount of water and thus, this process requires lower amount of water to carry out the water gas shift reaction compared to steam gasification. When the CaO adsorption was subsequently used for CO₂ capture, the simulation revealed that the CaO adsorption should be operated at carbonator temperature of 800 °C, CaO to biomass mass ratio of 1.78, and regenerator temperature of 900 °C. The integration of bagasse supercritical water gasification with CaO adsorption led to the production of green

hydrogen with a purity level of 99.98% and molar flow rate of 55.26 kmol/hr. Under the optimal operating conditions of all units, the energy efficiency is 26.01%.

Considering the quality and quantity of hydrogen and energy efficiency obtained from both processes, it can be concluded that green hydrogen production through steam bagasse gasification integrated with CaO adsorption demonstrates higher overall efficiency and achieves a slightly different purity compared to green hydrogen production through supercritical water bagasse gasification integrated with CaO adsorption. As a result, steam bagasse gasification integrated with CaO adsorption proves to be a suitable method for green hydrogen production.

6.2 Recommendations

- 1) Economics analysis should be considered to study the feasibility of the green hydrogen production.
- 2) Life cycle analysis (LCA) of green hydrogen production process should be considered to study the overall environmental impact of green hydrogen production.

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Table A.1 The simulation results of gasifier temperature in bagasse gasification at gasifier pressure of 1 bar and steam to biomass mass ratio of 0.1

Temperature (°C)	Mole Fraction			
	CO	CO ₂	CH ₄	H ₂
600	0.1255	0.1854	0.0689	0.3999
650	0.2096	0.1452	0.0445	0.4487
700	0.3027	0.0974	0.0275	0.4769
750	0.3810	0.0558	0.0167	0.4908
800	0.4316	0.0286	0.0104	0.4981
850	0.4587	0.0141	0.0067	0.5027
900	0.4720	0.0070	0.0044	0.5060
950	0.4784	0.0036	0.0030	0.5082
1000	0.4816	0.0020	0.0021	0.5098
1050	0.4833	0.0011	0.0015	0.5108
1100	0.4841	0.0007	0.0011	0.5116
1150	0.4846	0.0004	0.0008	0.5121
1200	0.4849	0.0003	0.0006	0.5124

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Table A.2 The simulation results of gasifier pressure in steam gasification of bagasse at gasifier temperature of 950 °C and steam to biomass mass ratio of 0.1

Pressure (bar)	Mole Fraction			
	CO	CO ₂	CH ₄	H ₂
1	0.4784	0.0036	0.0030	0.5082
2	0.4719	0.0071	0.0058	0.5032
3	0.4657	0.0103	0.0086	0.4983
4	0.4598	0.0134	0.0112	0.4936
5	0.4542	0.0163	0.0137	0.4891
6	0.4488	0.0192	0.0162	0.4847
7	0.4437	0.0219	0.0186	0.4805
8	0.4387	0.0244	0.0209	0.4764
9	0.4340	0.0269	0.0231	0.4724
10	0.4295	0.0293	0.0252	0.4686
11	0.4251	0.0316	0.0273	0.4648
12	0.4209	0.0338	0.0293	0.4612
13	0.4169	0.0359	0.0313	0.4577
14	0.4130	0.0379	0.0332	0.4543
15	0.4092	0.0399	0.0351	0.4509

เอกสารนี้เป็นเอกสารที่สงวนไว้สำหรับการใช้งานเพื่อการศึกษาเท่านั้น ไม่อนุญาตให้นำไปใช้ประโยชน์ด้านการค้า
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Table A.3 The simulation results in mole flow of steam to biomass mass ratio in steam gasification of bagasse at gasifier temperature of 950 °C, gasifier pressure of 1 bar

S/B	Mole Flow (kmol/hr)			
	CO	CO ₂	CH ₄	H ₂
0.1	34.97204	0.264994	0.216912	37.15154
0.2	35.48023	1.633962	0.035753	40.75998
0.3	33.64861	3.486888	0.014447	42.67682
0.4	32.00408	5.137408	0.008453	44.34533
0.5	30.52716	6.617115	0.005672	45.83338
0.6	29.19281	7.953039	0.004092	47.17404
0.7	27.98016	9.166693	0.00309	48.3907
0.8	26.87223	10.27531	0.002408	49.50136
0.9	25.85517	11.29286	0.001921	50.52037
1.0	24.91756	12.23083	0.001561	51.45942
1.1	24.04991	13.09875	0.001287	52.32816
1.2	23.24426	13.90461	0.001075	53.13467
1.3	22.49384	14.6552	0.000907	53.88575
1.4	21.7929	15.35628	0.000772	54.58724
1.5	21.13646	16.01282	0.000662	55.24412
1.6	20.52024	16.62913	0.000572	55.86069
1.7	19.9405	17.20895	0.000498	56.44073
1.8	19.39397	17.75554	0.000435	56.98751
1.9	18.87777	18.27179	0.000383	57.50392
2.0	18.38935	18.76026	0.000338	57.99252

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Table A.4 The simulation results in mole fraction of steam to biomass mass ratio in steam gasification of bagasse at gasifier temperature of 950 °C, gasifier pressure of 1 bar

S/B	Mole Fraction			
	CO	CO ₂	CH ₄	H ₂
0.1	0.4784	0.0036	0.0030	0.5082
0.2	0.4396	0.0202	0.0004	0.5050
0.3	0.3899	0.0404	0.0002	0.4945
0.4	0.3484	0.0559	0.0001	0.4827
0.5	0.3134	0.0679	0.0001	0.4705
0.6	0.2835	0.0772	0.0000	0.4581
0.7	0.2578	0.0845	0.0000	0.4459
0.8	0.2356	0.0901	0.0000	0.4339
0.9	0.2161	0.0944	0.0000	0.4223
1.0	0.1991	0.0977	0.0000	0.4111
1.1	0.1840	0.1002	0.0000	0.4003
1.2	0.1706	0.1020	0.0000	0.3899
1.3	0.1586	0.1033	0.0000	0.3799
1.4	0.1479	0.1042	0.0000	0.3704
1.5	0.1382	0.1047	0.0000	0.3612
1.6	0.1295	0.1049	0.0000	0.3525
1.7	0.1216	0.1049	0.0000	0.3441
1.8	0.1144	0.1047	0.0000	0.3360
1.9	0.1078	0.1043	0.0000	0.3283
2.0	0.1018	0.1038	0.0000	0.3209

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Table A.5 The simulation results in mole flow of water gas shift reactor temperature in steam gasification of bagasse at gasifier temperature of 950 °C, gasifier pressure of 1 bar, steam to biomass mass ratio of 0.1 and water to biomass mass ratio of 0.6

Temperature (°C)	Mole Flow (kmol/hr)			
	CO	CO ₂	CH ₄	H ₂
150	2.435247	32.80179	0.216912	69.68833
200	3.701889	31.53515	0.216912	68.42169
250	5.359338	29.8777	0.216912	66.76424
300	7.287183	27.94985	0.216912	64.83639
350	9.355309	25.88173	0.216912	62.76827
400	11.44766	23.78938	0.216912	60.67592

Table A.6 The simulation results in mole fraction of water gas shift reactor temperature in steam gasification of bagasse at gasifier temperature of 950 °C, gasifier pressure of 1 bar, steam to biomass mass ratio of 0.1 and water to biomass mass ratio of 0.6

Temperature (°C)	Mole Fraction			
	CO	CO ₂	CH ₄	H ₂
150	0.0229	0.3083	0.0020	0.6550
200	0.0348	0.2964	0.0020	0.6430
250	0.0504	0.2808	0.0020	0.6275
300	0.0685	0.2627	0.0020	0.6093
350	0.0879	0.2432	0.0020	0.5899
400	0.1076	0.2236	0.0020	0.5702

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Table A.7 The simulation results of water to biomass mass ratio in steam gasification of bagasse at gasifier temperature of 950 °C, gasifier pressure of 1 bar, steam to biomass mass ratio of 0.1 and water gas shift reactor temperature of 150 °C

Water/biomass	Mole Fraction			
	CO	CO ₂	CH ₄	H ₂
0.1	0.3691	0.0790	0.0028	0.5481
0.2	0.2791	0.1395	0.0026	0.5776
0.3	0.2003	0.1923	0.0024	0.6034
0.4	0.1312	0.2386	0.0023	0.6257
0.5	0.0707	0.2787	0.0022	0.6445
0.6	0.0229	0.3083	0.0020	0.6550
0.7	0.0056	0.3092	0.0019	0.6387
0.8	0.0026	0.2973	0.0018	0.6112
0.9	0.0016	0.2847	0.0018	0.5845
1.0	0.0012	0.2729	0.0017	0.5597
1.1	0.0009	0.2618	0.0016	0.5368
1.2	0.0007	0.2515	0.0016	0.5156
1.3	0.0006	0.2420	0.0015	0.4960
1.4	0.0005	0.2332	0.0014	0.4778
1.5	0.0004	0.2250	0.0014	0.4609

เอกสารนี้เป็นเอกสารที่สงวนไว้สำหรับการใช้งานเพื่อการศึกษาเท่านั้น ไม่อนุญาตให้นำไปใช้ประโยชน์ด้านการค้า
ไม่ว่ากรณีใดๆ ทั้งสิ้น อีกทั้งห้ามมิให้ดัดแปลงเนื้อหา และต้องอ้างอิงถึงเจ้าของเอกสารทุกครั้งที่มีการนำไปใช้

Table A.8 The simulation results of carbonator temperature in steam gasification of bagasse integrated with CaO adsorption at gasifier temperature of 950 °C, gasifier pressure of 1 bar, steam to biomass mass ratio of 0.1, calcium oxide to biomass mass ratio of 1.9 and regenerator temperature of 900 °C

Temperature (°C)	Mole Fraction			
	CO	CO ₂	CH ₄	H ₂
650	0.1057	0.0643	0.0465	0.6048
700	0.1348	0.0521	0.0185	0.6419
750	0.1508	0.0436	0.0060	0.6553
800	0.1589	0.0380	0.0018	0.6570
850	0.1639	0.0338	0.0006	0.6549

Table A.9 The simulation results of calcium oxide to biomass mass ratio in steam gasification of bagasse integrated with CaO adsorption at gasifier temperature of 950 °C, gasifier pressure of 1 bar, steam to biomass mass ratio of 0.1, carbonator temperature of 750 °C and regenerator temperature of 900 °C

CaO/Biomass	Mole fraction			
	CO	CO ₂	CH ₄	H ₂
0.1	0.2077	0.1120	0.0024	0.4810
0.2	0.2036	0.1043	0.0026	0.4966
0.3	0.1990	0.0965	0.0029	0.5129
0.4	0.1940	0.0887	0.0032	0.5301
0.5	0.1885	0.0810	0.0035	0.5482
0.6	0.1824	0.0733	0.0039	0.5673
0.7	0.1756	0.0657	0.0043	0.5875
0.8	0.1681	0.0582	0.0048	0.6088
0.9	0.1599	0.0508	0.0054	0.6314

เอกสารนี้เป็นเอกสารที่สงวนไว้สำหรับการใช้งานเพื่อการศึกษาเท่านั้น ไม่อนุญาตให้นำไปใช้ประโยชน์ด้านการค้า
ไม่ว่ากรณีใดๆ ทั้งสิ้น อีกทั้งห้ามมิให้ดัดแปลงเนื้อหา และต้องอ้างอิงถึงเจ้าของเอกสารทุกครั้งที่มีการนำไปใช้

Table A.9 The simulation results of calcium oxide to biomass mass ratio in steam gasification of bagasse integrated with CaO adsorption at gasifier temperature of 950 °C, gasifier pressure of 1 bar, steam to biomass mass ratio of 0.1, carbonator temperature of 750 °C and regenerator temperature of 900°C (Cont.)

CaO/Biomass	Mole fraction			
	CO	CO ₂	CH ₄	H ₂
1.0	0.1508	0.0436	0.0060	0.6553
1.1	0.1407	0.0367	0.0067	0.6808
1.2	0.1295	0.0301	0.0075	0.7079
1.3	0.1170	0.0238	0.0084	0.7368
1.4	0.1032	0.0179	0.0094	0.7677
1.5	0.0879	0.0127	0.0105	0.8009
1.6	0.0708	0.0080	0.0116	0.8367
1.7	0.0518	0.0043	0.0128	0.8754
1.8	0.0308	0.0016	0.0137	0.9178
1.9	0.0086	0.0001	0.0134	0.9653
2.0	0.0086	0.0001	0.0134	0.9653
2.1	0.0086	0.0001	0.0134	0.9653
2.2	0.0086	0.0001	0.0134	0.9653
2.3	0.0086	0.0001	0.0134	0.9653
2.4	0.0086	0.0001	0.0134	0.9653
2.5	0.0086	0.0001	0.0134	0.9653

เอกสารนี้เป็นเอกสารที่สงวนไว้สำหรับการใช้งานเพื่อการศึกษาเท่านั้น ไม่อนุญาตให้นำไปใช้ประโยชน์ด้านการค้า
ไม่ว่ากรณีใดๆ ทั้งสิ้น อีกทั้งห้ามมิให้ดัดแปลงเนื้อหา และต้องอ้างอิงถึงเจ้าของเอกสารทุกครั้งที่มีการนำไปใช้

Table A.10 Effect of regenerator temperature on the CO₂ mole flow rate released from CaCO₃ at a gasifier temperature of 950 °C, gasifier pressure of 1 bar, steam to biomass mass ratio of 0.1, calcium oxide to biomass mass ratio of 1.90, and carbonator temperature 750 °C

Temperature (°C)	Mole Flow of CO ₂ (kmol/hr)
400	0.0000
450	0.0000
500	0.0000
550	0.0000
600	0.0000
650	0.0000
700	0.0000
750	0.0000
800	0.0000
850	0.0000
900	33.8817
950	33.8817
1000	33.8817
1050	33.8817
1100	33.8817
1150	33.8817
1200	33.8817
1250	33.8817
1300	33.8817
1350	33.8817
1400	33.8817

เอกสารนี้เป็นเอกสารที่สงวนไว้สำหรับการใช้งานเพื่อการศึกษาเท่านั้น ไม่อนุญาตให้นำไปใช้ประโยชน์ด้านการค้า
ไม่ว่ากรณีใดๆ ทั้งสิ้น อีกทั้งห้ามมิให้ดัดแปลงเนื้อหา และต้องอ้างอิงถึงเจ้าของเอกสารทุกครั้งที่มีการนำไปใช้



เอกสารนี้เป็นเอกสารที่สงวนไว้สำหรับการใช้งานเพื่อการศึกษาเท่านั้น ไม่อนุญาตให้นำไปใช้ประโยชน์ด้านการค้า
ไม่ว่ากรณีใดๆ ทั้งสิ้น อีกทั้งห้ามมิให้ดัดแปลงเนื้อหา และต้องอ้างอิงถึงเจ้าของเอกสารทุกครั้งที่มีการนำไปใช้

Table B.1 The simulation results of gasifier temperature in supercritical water gasification of bagasse at gasifier pressure of 221 bar and supercritical water to biomass mass ratio of 0.4

Temperature (°C)	Mole Fraction			
	CO	CO ₂	CH ₄	H ₂
375	0.0001	0.1499	0.1671	0.0044
400	0.0002	0.1634	0.1797	0.0063
425	0.0003	0.1747	0.1899	0.0087
450	0.0006	0.1844	0.1981	0.0118
475	0.0010	0.1928	0.2049	0.0154
500	0.0017	0.2001	0.2102	0.0199
525	0.0026	0.2064	0.2142	0.0251
550	0.0040	0.2117	0.2171	0.0312
575	0.0058	0.2161	0.2189	0.0381
600	0.0084	0.2196	0.2197	0.0460
625	0.0118	0.2222	0.2194	0.0549
650	0.0162	0.2238	0.2181	0.0647
675	0.0219	0.2243	0.2160	0.0755
700	0.0290	0.2238	0.2129	0.0872
725	0.0377	0.2220	0.2090	0.0998
750	0.0481	0.2190	0.2043	0.1132
775	0.0605	0.2148	0.1989	0.1274
800	0.0750	0.2091	0.1928	0.1422
825	0.0915	0.2022	0.1861	0.1576
850	0.1100	0.1939	0.1789	0.1734
875	0.1305	0.1844	0.1712	0.1895
900	0.1526	0.1738	0.1632	0.2058
925	0.1762	0.1623	0.1549	0.2221

เอกสารนี้เป็นเอกสารที่สงวนไว้สำหรับการใช้งานเพื่อการศึกษาเท่านั้น ไม่อนุญาตให้นำไปใช้ประโยชน์ด้านการค้า
ไม่ว่ากรณีใดๆ ทั้งสิ้น อีกทั้งห้ามมิให้ดัดแปลงเนื้อหา และต้องอ้างอิงถึงเจ้าของเอกสารทุกครั้งที่มีการนำไปใช้

Table B.1 The simulation results of gasifier temperature in supercritical water gasification of bagasse at gasifier pressure of 221 bar and steam to biomass mass ratio of 0.4 (Cont.)

Temperature (°C)	Mole Fraction			
	CO	CO ₂	CH ₄	H ₂
950	0.2007	0.1502	0.1465	0.2384
975	0.2259	0.1375	0.1380	0.2545
1000	0.2512	0.1247	0.1295	0.2703
1025	0.2695	0.1125	0.1171	0.2882
1050	0.2832	0.1014	0.1032	0.3069
1075	0.2956	0.0915	0.0902	0.3249
1100	0.3067	0.0827	0.0782	0.3419
1125	0.3166	0.0749	0.0671	0.3578
1150	0.3253	0.0681	0.0572	0.3724
1175	0.3329	0.0622	0.0482	0.3857
1200	0.3395	0.0571	0.0404	0.3975

เอกสารนี้เป็นเอกสารที่สงวนไว้สำหรับการใช้งานเพื่อการศึกษาเท่านั้น ไม่อนุญาตให้นำไปใช้ประโยชน์ด้านการค้า
ไม่ว่ากรณีใดๆ ทั้งสิ้น อีกทั้งห้ามมิให้ดัดแปลงเนื้อหา และต้องอ้างอิงถึงเจ้าของเอกสารทุกครั้งที่มีการนำไปใช้

Table B.2 The simulation results of gasifier pressure in supercritical water gasification of bagasse at gasifier temperature of 1200 °C and supercritical water to biomass mass ratio of 0.4

Pressure (bar)	Mole Fraction			
	CO	CO ₂	CH ₄	H ₂
221	0.3395	0.0571	0.0404	0.3975
241	0.3369	0.0589	0.0444	0.3905
261	0.3344	0.0607	0.0484	0.3838
281	0.3319	0.0624	0.0522	0.3774
301	0.3295	0.0641	0.0559	0.3712
321	0.3272	0.0658	0.0594	0.3653
341	0.3249	0.0674	0.0628	0.3596
350	0.3239	0.0681	0.0643	0.3571

Table B.3 The simulation results in mole flow of supercritical water to biomass mass ratio in supercritical water gasification of bagasse at gasifier temperature of 1200 °C and gasifier pressure of 221 bar

SCW/Biomass	Mole Flow (kmol/hr)			
	CO	CO ₂	CH ₄	H ₂
0.1	24.87009	2.568011	4.413156	23.26313
0.2	28.71462	2.976384	5.04195	26.66682
0.3	29.04273	3.915474	4.191742	30.57353
0.4	28.86404	4.854369	3.431533	33.79305
0.5	28.56558	5.744212	2.840155	36.45703
0.6	28.18933	6.588166	2.37245	38.70409
0.7	27.76289	7.389128	1.997924	40.62863
0.8	27.30526	8.149752	1.694937	42.29822

เอกสารนี้เป็นเอกสารที่สงวนไว้สำหรับการใช้งานเพื่อการศึกษาเท่านั้น ไม่อนุญาตให้นำไปใช้ประโยชน์ด้านการค้า
ไม่ว่ากรณีใดๆ ทั้งสิ้น อีกทั้งห้ามมิให้ดัดแปลงเนื้อหา และต้องอ้างอิงถึงเจ้าของเอกสารทุกครั้งที่มีการนำไปใช้

Table B.3 The simulation results in mole flow of supercritical water to biomass mass ratio in supercritical water gasification of bagasse at gasifier temperature of 1200 °C and gasifier pressure of 221 bar (Cont.)

SCW/Biomass	Mole Flow (kmol/hr)			
	CO	CO ₂	CH ₄	H ₂
0.9	26.82979	8.872512	1.447642	43.76286
1.0	26.34601	9.559746	1.24419	45.06045
1.1	25.8607	10.21367	1.075578	46.22021
1.2	25.37869	10.83637	0.934884	47.265
1.3	24.90337	11.42984	0.816736	48.21291
1.4	24.43709	11.99594	0.716923	49.07844
1.5	23.98142	12.5364	0.632123	49.87331
1.6	23.53738	13.05287	0.559691	50.60708
1.7	23.10557	13.54686	0.497512	51.2876
1.8	22.68629	14.01978	0.44388	51.92141
1.9	22.27961	14.47293	0.39741	52.51398
2.0	21.88544	14.90753	0.356975	53.06989

เอกสารนี้เป็นเอกสารที่สงวนไว้สำหรับการใช้งานเพื่อการศึกษาเท่านั้น ไม่อนุญาตให้นำไปใช้ประโยชน์ด้านการค้า
ไม่ว่ากรณีใดๆ ทั้งสิ้น อีกทั้งห้ามมิให้ดัดแปลงเนื้อหา และต้องอ้างอิงถึงเจ้าของเอกสารทุกครั้งที่มีการนำไปใช้

Table B.4 The simulation results in mole fraction of supercritical water to biomass mass ratio in supercritical water gasification of bagasse at gasifier temperature of 1200 °C and gasifier pressure of 221 bar

SCW/Biomass	Mole Fraction			
	CO	CO ₂	CH ₄	H ₂
0.1	0.4070	0.0420	0.0722	0.3807
0.2	0.4086	0.0424	0.0717	0.3794
0.3	0.3726	0.0502	0.0538	0.3922
0.4	0.3395	0.0571	0.0404	0.3975
0.5	0.3113	0.0626	0.0310	0.3973
0.6	0.2870	0.0671	0.0242	0.3940
0.7	0.2656	0.0707	0.0191	0.3887
0.8	0.2467	0.0736	0.0153	0.3821
0.9	0.2298	0.0760	0.0124	0.3749
1.0	0.2147	0.0779	0.0101	0.3673
1.1	0.2011	0.0794	0.0084	0.3595
1.2	0.1888	0.0806	0.0070	0.3516
1.3	0.1776	0.0815	0.0058	0.3439
1.4	0.1674	0.0822	0.0049	0.3363
1.5	0.1581	0.0827	0.0042	0.3288
1.6	0.1496	0.0829	0.0036	0.3216
1.7	0.1417	0.0831	0.0031	0.3146
1.8	0.1345	0.0831	0.0026	0.3078
1.9	0.1278	0.0830	0.0023	0.3012
2.0	0.1216	0.0828	0.0020	0.2949

เอกสารนี้เป็นเอกสารที่สงวนไว้สำหรับการใช้งานเพื่อการศึกษาเท่านั้น ไม่อนุญาตให้นำไปใช้ประโยชน์ด้านการค้า
ไม่ว่ากรณีใดๆ ทั้งสิ้น อีกทั้งห้ามมิให้ดัดแปลงเนื้อหา และต้องอ้างอิงถึงเจ้าของเอกสารทุกครั้งที่มีการนำไปใช้

Table B.5 The simulation results in mole fraction of water gas shift reactor temperature in supercritical water gasification of bagasse at gasifier temperature of 1200 °C, gasifier pressure of 221 bar, steam to biomass mass ratio of 0.4 and water to biomass mass ratio of 0.2

Temperature (°C)	Mole Fraction			
	CO	CO ₂	CH ₄	H ₂
150	0.0445	0.3063	0.0357	0.6075
200	0.0533	0.2975	0.0357	0.5986
250	0.0667	0.2841	0.0357	0.5852
300	0.0834	0.2674	0.0357	0.5685
350	0.1019	0.2489	0.0357	0.5500
400	0.1209	0.2299	0.0357	0.5310

Table B.6 The simulation results in mole flow of water gas shift reactor temperature in supercritical water gasification of bagasse at gasifier temperature of 1200 °C, gasifier pressure of 221 bar, steam to biomass mass ratio of 0.4 and water to biomass mass ratio of 0.2

Temperature (°C)	Mole Flow (kmol/hr)			
	CO	CO ₂	CH ₄	H ₂
150	4.276991	29.44142	3.431533	58.3801
200	5.120161	28.59825	3.431533	57.53693
250	6.411898	27.30651	3.431533	56.24519
300	8.018265	25.70015	3.431533	54.63883
350	9.793803	23.92461	3.431533	52.86329
400	11.61805	22.10036	3.431533	51.03904

เอกสารนี้เป็นเอกสารที่สงวนไว้สำหรับการใช้งานเพื่อการศึกษาเท่านั้น ไม่อนุญาตให้นำไปใช้ประโยชน์ด้านการค้า
ไม่ว่ากรณีใดๆ ทั้งสิ้น อีกทั้งห้ามมิให้ดัดแปลงเนื้อหา และต้องอ้างอิงถึงเจ้าของเอกสารทุกครั้งที่มีการนำไปใช้

Table B.7 The simulation results of water to biomass mass ratio in steam gasification of bagasse at gasifier temperature of 1200 °C, gasifier pressure of 221 bar, supercritical water to biomass mass ratio of 0.4 and water gas shift reactor temperature of 150 °C

Water/biomass	Mole Fraction			
	CO	CO ₂	CH ₄	H ₂
0.2	0.0445	0.3063	0.0357	0.6075
0.3	0.0092	0.3225	0.0338	0.6072
0.4	0.0032	0.3113	0.0320	0.5813
0.5	0.0018	0.2973	0.0304	0.5539
0.6	0.0012	0.2838	0.0290	0.5284
0.7	0.0009	0.2713	0.0277	0.5050
0.8	0.0007	0.2599	0.0265	0.4835
0.9	0.0006	0.2493	0.0254	0.4637
1.0	0.0005	0.2395	0.0244	0.4455
1.1	0.0004	0.2305	0.0235	0.4286
1.2	0.0003	0.2221	0.0226	0.4129
1.3	0.0003	0.2142	0.0218	0.3984
1.4	0.0003	0.2070	0.0211	0.3848
1.5	0.0002	0.2002	0.0204	0.3721

เอกสารนี้เป็นเอกสารที่สงวนไว้สำหรับการใช้งานเพื่อการศึกษาเท่านั้น ไม่อนุญาตให้นำไปใช้ประโยชน์ด้านการค้า
ไม่ว่ากรณีใดๆ ทั้งสิ้น อีกทั้งห้ามมิให้ดัดแปลงเนื้อหา และต้องอ้างอิงถึงเจ้าของเอกสารทุกครั้งที่มีการนำไปใช้

Table B.8 The simulation results of carbonator temperature in steam gasification of bagasse integrated with CaO adsorption at gasifier temperature of 1200 °C, gasifier pressure of 221 bar, supercritical water to biomass mass ratio of 0.4, calcium oxide to biomass mass ratio of 1.78 and regenerator temperature of 900 °C

Temperature (°C)	Mole Fraction			
	CO	CO ₂	CH ₄	H ₂
650	0.1277	0.0584	0.0747	0.6046
700	0.1653	0.0423	0.0355	0.6537
750	0.1877	0.0317	0.0137	0.6793
800	0.1985	0.0258	0.0047	0.6884
850	0.2038	0.0223	0.0016	0.6900

Table B.9 The simulation results of calcium oxide to biomass mass ratio in steam gasification of bagasse integrated with CaO adsorption at gasifier temperature of 1200 °C, gasifier pressure of 221 bar, supercritical water to biomass mass ratio of 0.4, carbonator temperature of 800 °C and regenerator temperature of 900 °C

CaO/Biomass	Mole fraction			
	CO	CO ₂	CH ₄	H ₂
0.10	0.2592	0.0900	0.0012	0.4928
0.20	0.2550	0.0824	0.0013	0.5101
0.30	0.2504	0.0748	0.0015	0.5284
0.40	0.2452	0.0674	0.0017	0.5477
0.50	0.2394	0.0600	0.0020	0.5680
0.60	0.2330	0.0527	0.0023	0.5895
0.70	0.2257	0.0456	0.0027	0.6122
0.80	0.2177	0.0388	0.0032	0.6362

เอกสารนี้เป็นเอกสารที่สงวนไว้สำหรับการใช้งานเพื่อการศึกษาเท่านั้น ไม่อนุญาตให้นำไปใช้ประโยชน์ด้านการค้า
ไม่ว่ากรณีใดๆ ทั้งสิ้น อีกทั้งห้ามมิให้ดัดแปลงเนื้อหา และต้องอ้างอิงถึงเจ้าของเอกสารทุกครั้งที่มีการนำไปใช้

Table B.9 The simulation results of calcium oxide to biomass mass ratio in steam gasification of bagasse integrated with CaO adsorption at gasifier temperature of 1200 °C, gasifier pressure of 221 bar, supercritical water to biomass mass ratio of 0.4, carbonator temperature of 800 °C and regenerator temperature of 900 °C (Cont.)

CaO/Biomass	Mole fraction			
	CO	CO ₂	CH ₄	H ₂
0.90	0.2087	0.0321	0.0038	0.6616
1.00	0.1985	0.0258	0.0047	0.6884
1.10	0.1871	0.0199	0.0058	0.7167
1.20	0.1740	0.0145	0.0075	0.7464
1.30	0.1588	0.0097	0.0102	0.7773
1.40	0.1404	0.0056	0.0148	0.8087
1.50	0.1169	0.0027	0.0233	0.8388
1.60	0.0852	0.0009	0.0386	0.8658
1.70	0.0437	0.0002	0.0619	0.8902
1.78	0.0028	0.0000	0.0862	0.9097
1.80	0.0028	0.0000	0.0862	0.9097
1.90	0.0028	0.0000	0.0862	0.9097
2.00	0.0028	0.0000	0.0862	0.9097
2.10	0.0028	0.0000	0.0862	0.9097
2.20	0.0028	0.0000	0.0862	0.9097
2.30	0.0028	0.0000	0.0862	0.9097
2.40	0.0028	0.0000	0.0862	0.9097
2.50	0.0028	0.0000	0.0862	0.9097

เอกสารนี้เป็นเอกสารที่สงวนไว้สำหรับการใช้งานเพื่อการศึกษาเท่านั้น ไม่อนุญาตให้นำไปใช้ประโยชน์ด้านการค้า
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Table B.10 Effect of regenerator temperature on the CO₂ mole flowrate released from CaCO₃ at a gasifier temperature of 1200 °C, gasifier pressure of 221 bar, supercritical water to biomass mass ratio of 0.4, calcium oxide to biomass mass ratio of 1.78, and carbonator temperature of 800 °C

Temperature (°C)	Mole Flowrate ofCO2 (kmoI/hr)
400	0.0000
450	0.0000
500	0.0000
550	0.0000
600	0.0000
650	0.0000
700	0.0000
750	0.0000
800	0.0000
850	0.0000
900	31.7418
950	31.7418
1000	31.7418
1050	31.7418
1100	31.7418
1150	31.7418
1200	31.7418
1250	31.7418
1300	31.7418
1350	31.7418
1400	31.7418

เอกสารนี้เป็นเอกสารที่สงวนไว้สำหรับการใช้งานเพื่อการศึกษาเท่านั้น ไม่อนุญาตให้นำไปใช้ประโยชน์ด้านการค้า
ไม่ว่ากรณีใดๆ ทั้งสิ้น อีกทั้งห้ามมิให้ดัดแปลงเนื้อหา และต้องอ้างอิงถึงเจ้าของเอกสารทุกครั้งที่มีการนำไปใช้

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เอกสารนี้เป็นเอกสารที่สงวนไว้สำหรับการใช้งานเพื่อการศึกษาเท่านั้น ไม่อนุญาตให้นำไปใช้ประโยชน์ด้านการค้า
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