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Modelling of Wood Biomass Gasification for Process Optimization

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ABSTRACT

Biomass gasification is a promising technology for sustainable energy production. To date, extensive research has been conducted on biomass gasification, particularly focusing on the reaction models of the process. However, existing models are too complex to apply to the control system or to optimize the process operating conditions effectively, limiting their practical use for industrial applications. To address this, a simple reaction model for biomass gasification was developed and validated. A steady state simulation of the biomass gasification process is conducted to analyze gasifier behavior and provide insights into reaction dynamic. The findings in this study align well with existing literature, confirming the reliability of the approach. This simulation serves as a foundation for further study in process control and optimization. Future work will include experimental validation to enhance model accuracy and applicability.

Keywords: Biomass, Modelling and Simulations, Gasification

INTRODUCTION

The urgency to tackle environmental challenges such as climate change, pollution, and resource depletion has become increasingly evident. As a result of the consequences of unsustainable practices, technology offering innovative solutions to mitigate environmental degradation and foster long-term resilience has garnered significant public attention.

Biomass gasification appears to be such a technological innovation, offering a sustainable alternative to traditional energy generation methods. It is one of the most effective technologies which has great potential for biomass energy recovery. Biomass gasification converts biomass into syngas (CH_4, CO, H_2 and CO_2) which can be further converted into electricity and biofuel [1], [2]. This technology aligns with the global shift toward sustainable development by promoting waste utilization and reducing carbon footprint.

There is a wide variety of biomass feedstock, including agriculture, forestry residue and municipal waste. Among all these biomass, woody biomass has shown great potential as a good-quality feedstock due to its high energy content and relatively high fixed carbon content [3]. Japan's forest covers about 25 million hectares, which accounts for two-thirds of the country's land. Approximately 40% of the forest planted, predominantly with Japanese cedar (Cryptomeria japonica), is valued for its adaptability and growth, but its pollen causes allergies affecting 40% of the population. Thus, Japan government implement measures in 2024 to reduce pollen dispersal by promoting sustainable wood utilization [4].

With the growing interest in biomass gasification, numerous studies have been conducted to study this multifaceted and complicated process focusing on areas such as modelling, optimization, process analysis and gasifier design [5]. Mathematical models can be an effective tool to evaluate the plant's performance, optimize its operation and improve its efficiency [6]. These reaction models enable more computationally efficient predictions of the yield and composition of various gas and tar species, making it feasible to simulate complex reactor configurations without compromising accuracy. Most of the simulation studies focus on thermodynamic equilibrium modelling. Many researchers have found a high degree of similarity between modelling and theoretical predictions based on equilibrium modelling [7]–[9].

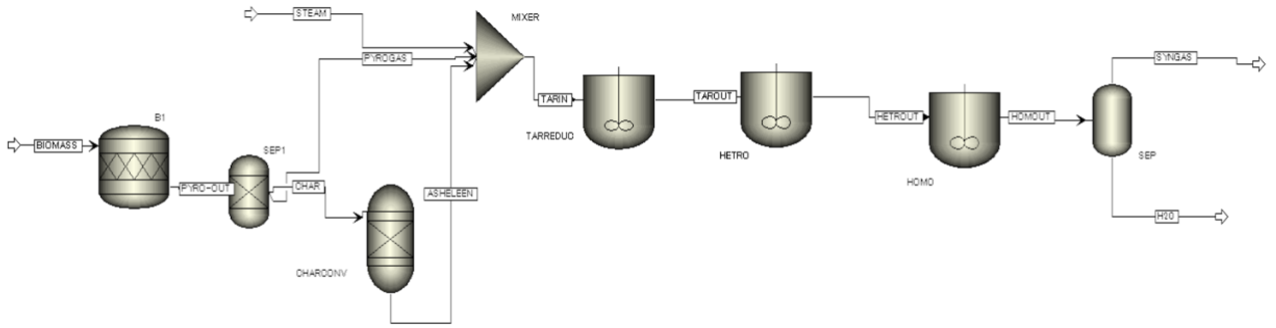

Figure 1: Flow chart of biomass gasification simulation using Aspen Plus

However, for dynamic simulations and control applications, a model which able to capture the time-dependent behaviour of the process is necessary. This model needs to employ reaction kinetic to capture the time-dependent evolution of the process.

Several authors discuss the kinetic model of steam gasification on wood biomass especially on pyrolysis [10] - [14]. However, the existing models are too complex and not suitable to apply to the control system or to optimize the process operating conditions effectively, limiting their practical use for industrial applications.

To overcome this limitation, the present paper aims to bridge this gap by creating a kinetic model to investigate wood biomass gasification.

MATERIALS AND METHOD

Biomass samples

Japanese waste wood was chosen as a feedstock for this biomass gasification simulation. The proximate and ultimate value of the biomass used in this research is presented in Table 1.

Table 1: Proximate and ultimate analysis of feedstock

Proximate analysis wt.%	**Japanese Waste Wood [10]**
Moisture Content (as determined basis)	21.8 ± 7.5
Volatile Material (dry basis)	84 ± 4.1
Fixed Carbon (dry basis)	51.4 ± 2
Ultimate analysis, wt.% (dry ash free basis)	
C	51.4 ± 0.2
H	6.2 ± 0.3
N	0.3 ± 0.3
O	42.2 ± 2.1
HHV, MJ/kg	21.1 ± 0.9

Process Assumption

There are a few assumptions considered in this process modelling:

- Temperature and pressure drop in processes are neglected.
- Ash is inert and does not participate in the reaction.

Modelling and Simulation Software

The biomass gasification discussed in this paper is based on uncoupling the downdraft biomass gasifier into different parts based on the main reactions, biomass pyrolysis and reduction. These parts are linked with different types of reactors in Aspen Plus version 14.

The Peng-Robinson-Boston-Mathias (PB-RM) property method is used in this simulation. This method is recommended for hydrocarbon processing applications such as gas processing in all temperatures and pressures [16]. Biomass, Char and Ash were defined as non-conventional components in this process. The enthalpy and density models used for the non-conventional components were DCOALIGT and HCOALGEN. The stream classes defined as MIXCINC.

Aspen Plus Model Description

The wood biomass gasification flowsheet has been developed as shown in Figure 1 while the unit operation blocks used in the flowsheet are summarized and presented in Table 2.

The feed stream “Biomass” was dry basis biomass, specified as a non-conventional stream with the proximate and ultimate analysis value as shown in Table 1. The mass flow rate was set as 50kg/hr. The biomass was directly fed to pyrolysis reactor “B1” as the temperature of the feed stream was higher than the wood drying temperature [17]. Pyrolysis is a complicated thermochemical process. It can be modelled by a stoichiometric reactor to simulate the reaction based on the following empirical equations in Table 3 where $Y_i = aT^2 + bT + c$, [kg h^{-1}] is a

Table 2: Reactor block description used in the simulation

Default ID	Assigned ID	Operating Condition	Description
RStoic	B1	1 atm 850 °C	Stoichiometric reactor - model the reactor with specified reaction extends or conversion
SEP2	SEP1	1 atm 850 °C	Separator – separate char from pyrolysis gases
	SEP	1 atm 850 °C	Separator – separate water from syngas
RYield	CHAR-CONV	1 atm 850 °C	Yield reactor – convert char into its conventional element according to yield distribution data
Mixer	MIXER	1 atm 850 °C	Mixer - Mixing steam and gases
RCSTR	TARREDUC	1 atm 850 °C	Continuous stirred tank reactor – tar reduction take place
	HETRO	1 atm 850 °C	Continuous stirred tank reactor – heterogenous gasification take place
	HOMO	1 atm 850 °C	Continuous stirred tank reactor – homogenous gasification take place

Table 3: Empirical correlations of wood chips pyrolysis [18]

i	a	b	c
CH_4	-4.341×10^{-5}	10.12×10^{-2}	-51.08
H_2	1.362×10^{-5}	-2.517×10^{-2}	12.19
CO	-3.524×10^{-5}	9.770×10^{-2}	-24.93
CO_2	3.958×10^{-5}	-9.126×10^{-2}	64.02
C_2H_4	-6.873×10^{-5}	14.94×10^{-2}	-76.89
C_2H_6	8.265×10^{-6}	-2.105×10^{-2}	13.38
C_6H_6	-3.134×10^{-5}	7.544×10^{-2}	-42.72
C_7H_8	-4.539×10^{-5}	0.687×10^{-2}	1.462
C_6H_6O	1.508×10^{-5}	-3.662×10^{-2}	22.19
$C_{10}H_8$	-8.548×10^{-6}	1.882×10^{-2}	-9.851
H_2O	5.157×10^{-5}	11.86×10^{-2}	84.91

mass yield of pyrolysis product, T [K] is a reaction temperature, and a [kg h^{-1} K^{-2}], b [kg h^{-1} K^{-1}], and c [kg h^{-1}] are coefficients obtained from experimental data. This empirical model can be applied for the reactor temperature between 700 and 1000 °C [18]. This empirical equation is a simplified method to present the yield of pyrolysis including the primary and secondary tar. The char mass yield is calculated based on mass balances after other product determinations. The pyrolysis gas is then introduced into a separator "SEP 1" to separate the char. The char is turned into conventional elements according to its yield distribution data at "CHARCONV" reactor. The gas produced is mixed with pyrolysis gases and steam at "MIXER". The gases undergo tar reduction with the reaction R3 listed in Table 4. Following tar treatment, the gases were introduced into the 'HETRO' reactor to undergo a heterogeneous gasification process at 850 °C and 1 bar, facilitated by reaction R1. Subsequently, homogenous gasification was conducted under the same pressure and temperature at "HOMO" reactor with reaction R2.

Table 4: List of reactions involved

No	Reaction	Kinetic	Source
R1	$C + CO_2 \leftrightarrow 2CO$	$4.4Te^{(\frac{-1.62\times10^8}{RT})}[CO_2]^{0.6}$	[1]
	$C + H_2O \leftrightarrow CO + H_2$	$1.33Te^{(\frac{-1.47\times10^8}{RT})}[H_2O]^{0.6}$	[1]
R2	$CH_4 + H_2O \rightarrow CO + 3H_2$	$3.0 \times 10^5 e^{(\frac{1.25\times10^8}{RT})}[CH_4]^1[O_2]^1$	[23]
	$CO + H_2O \rightarrow CO_2 + H_2$	$2.78 \times 10^6 e^{(\frac{-1.26\times10^7}{RT})}\left([CO][H_2O]\text{-}\ \frac{[CO][H_2O]}{k_p(T)}\right)$ $k_p(T) = 0.0265e^{(\frac{4.55\times10^7}{RT})}$	[1]
R3	$C_6H_6 + 2H_2O \rightarrow 3C + 2CH_4 + 2CO$	$4.0 \times 10^{16} e^{(\frac{-4.43\times10^5}{RT})}[C_6H_6]^{1.3}[H_2]^{-0.4}[H_2O]^{0.2}$	[18]
	$C_7H_8 + H_2 \rightarrow C_6H_6 + CH_4$	$1.04 \times 10^{12} e^{(\frac{-2.47\times10^5}{RT})}[C_7H_8]^1[H_2]^{0.5}$	[18]
	$C_6H_6O \rightarrow CO + 0.4C_{10}H_8 + 0.15C_6H_6 + 0.1CH_4 + 0.75H_2$	$10^7 e^{(\frac{10^5}{RT})}[C_6H_6O]^1$	[18]
	$C_{10}H_8 \rightarrow 9C + 0.16667C_6H_6 + 3.5H_2$	$3.4 \times 10^{14} e^{(\frac{3.5\times10^5}{RT})}[C_{10}H_8]^{1.6}[H_2]^{-0.5}$	[18]

RESULT AND DISCUSSION

Effect of temperature on syngas composition

Figure 2 presents the effect of temperature on the syngas composition at a steam-to-biomass ratio of 3. The temperature was varied in the range of 750 ˚C to 1050 ˚C as the suitable temperature for gasification to occur is more than 750 ˚C [19].

Raising the temperature increases the yield of H_2 and decreases the contents of CO_2 and CH_4. H2 has increased 36% from 750 ˚C to 1050 ˚C. This result is almost consistent with the results by Talero et al. in 2022 [15]. In particular, similar CO synthesis trend was also reported in several previous papers [9], [20], [21].

From the R1 and R2 reactions listed in Table 4, only the water gas shift reaction is exothermic. When increasing the temperature of the gasification, Boudourd reaction, water gas reaction and steam methane reforming which are endothermic reactions favour the forward reaction, resulting in an increase in H_2 and CO composition and decreasing in CH_4 and C composition. The exothermic properties of the water gas shift reaction hinder the production of H_2 and CO_2.

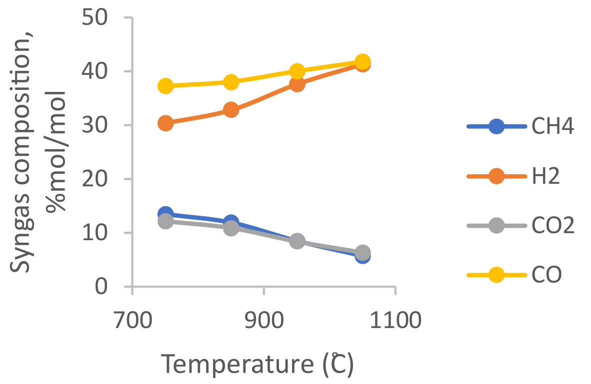

Figure 2: Effect of temperature on syngas composition

Effect of steam to biomass ratio on syngas composition

The effect of steam to biomass ratio is one of the critical parameters that affect gasification efficiency, syngas composition and reaction mechanism. Figure 3 shows the effect of steam to biomass ratio on the syngas composition at a gasification temperature of 850 ˚C. There is a slight increase in the H_2 value when increasing the steam-to-biomass ratio. This can be explained according to Le Chatelier's Principle as the increase in the steam will favour the H_2 formation reaction, especially in steam methane reforming and water gas reaction. CH_4 and CO will decrease to maintain the equilibrium of the reaction. A similar result is obtained by Huang where the syngas composition is studied from the range of 0.5 to 3.0 [22] whereas a similar increasing trend is also discussed by Paiva and Florin with lower steam-to-biomass ratio [7], [21].

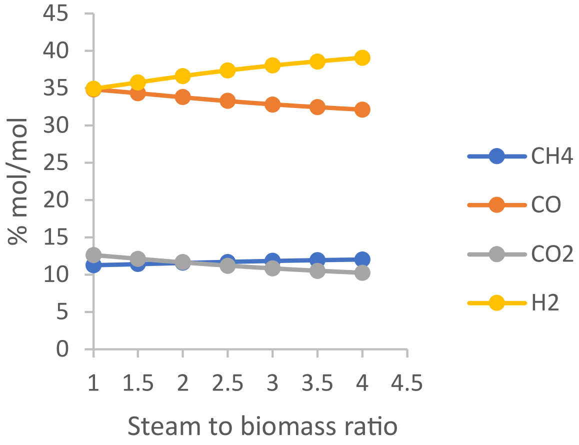

Figure 3: Effect of steam to biomass ratio on syngas composition

The introduction of steam during the gasification process promotes the further pyrolysis and gasification of tar and coke. This can improve the syngas quality as shown in Figure 4.

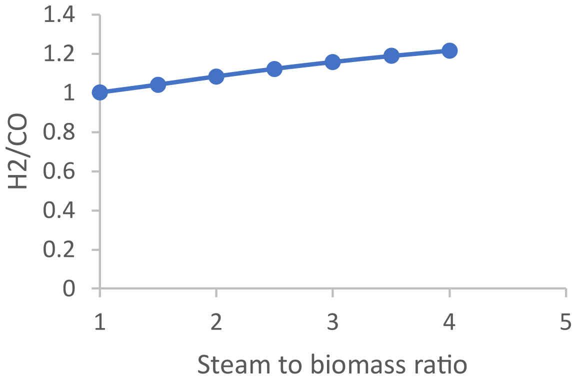

Figure 4: Effect of steam to biomass ratio on H2/CO ratio

It can be seen that the proposed kinetic biomass gasification models showed the consistent results with the previous research. From these results, the authors concluded that the proposed models capture the characteristics of the gasification reaction, although the proposed models are much simpler than others counterparts. Furthermore, it can be said that the control system can be designed based on these models for optimizing the process operation.

CONCLUSION

A simple kinetic biomass gasification model is developed in the Aspen Plus simulator to discuss the syngas production during the steam gasification of Japan waste wood. Each kinetic reaction captured in the model affects the biomass gasification process.

In this study, we compared our simulation model with those presented in previous research to assess its relative performance and validity. This study helps develop a control system in future studies which able to capture the complex interactions between the factors that influence the performance of gasifiers and optimize them for improved efficiency and scalability in industrial applications.

While our current analysis is based on simplified models, we recognize the importance of validating these findings through experimental data. Therefore, in future work, we plan to conduct experiments which will allow us to rigorously compare our simplified models with experimental outcomes, ensuring greater accuracy and reliability in our conclusions.

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