

Kinetic Modelling of Wood Biomass Gasification for Process Optimization

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Biomass gasification is a sustainable thermochemical process to produce syngas, offering a renewable alternative to fossil fuel. To date, many studies have been conducted on biomass gasification, particularly focusing on the reaction models of the process. However, existing models are too complex to be applied to control systems 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 in this research. This study presents a simple kinetic-based biomass gasification model developed in a commercial process simulator, Aspen Plus using Japanese Cypress as feedstock. The process was divided into three main parts, pyrolysis, tar cracking, and char reduction stages. Syngas yield trends on gasification temperature and steam to biomass ratio were studied. At around 900 °C, the proposed gasification system produced the highest CO and lowest CO₂ concentrations, indicating it as the optimal gasification temperature. These results show consistent trends with the literature, validating the model's practical applicability. This study also serves as a foundation for further study in process control and optimization.

1. Introduction

In Japan, the forests cover about 250 Gm², roughly two-thirds of its total land area (Forestry Agency, 2023). Out of this, the plantation forests account for 100 Gm². 70 % of the plantation forest is primarily composed of Japanese cypress and cedar. However, the prevalence rate of Japanese cedar and cypress pollinosis in Japan has been increasing steadily by 10 % every decade for the past 20 years. Pollen allergies have affected 42.5 % of people in Japan, and 38.8 % are sensitive to cedar pollen (Speed, 2025). Studies show that the age of the tree is one of the reasons pollen production increases after the 20th year. To overcome this issue, the Japanese government promotes the cutting and use of wood plantations that release pollen and replanting them with low-pollen species.

In recent decades, the research area of wood biomass gasification has focused on tar reduction and catalyst innovation, production of hydrogen-rich syngas and kinetic modelling and simulation. In Aspen Plus, pyrolysis reactions are typically modelled using an RYield reactor, while gasification reactions are often represented with an RGibbs reactor. Han et al. (2017) studied on the biomass gasification by simulating it with a single Gibbs reactor while Saharian et al. (2021) separated the gasification process into 2 Gibbs reactors (combustion and reduction). For the combustion process, minimum air will be supplied to the reactor. Cao et al. (2019) also carried out biomass gasification reaction with air as the gasifying agent. Similar to Saharian et al. (2021), Cao et al. (2019) separated the biomass gasification into 2 processes (volatile material combustion and char reduction). However, Cao et al. (2019) used Gibbs reactor for volatile material combustion and continuous stir tank reactor for char reduction. For kinetic-based simulation of biomass gasification, the estimation of the syngas composition is based on the reaction rates within the residence time or volume. Aspen Plus offers two types of unit blocks for the chemical kinetic reactions, which are continuous stirring tank reactor and plug flow reactor. Several researchers have discussed this method by integrating the reactor with an Excel subroutine (Puig-Gamero et al., 2021) or MATLAB for the modelling process (Rabea et al., 2022). Others focus on the pyrolysis kinetics of lignocellulosic biomass, involving multiple parallel and consecutive reactions (Humbird et al., 2017) which increase computational intensity. Peters et al. (2017) simulated the wood pyrolysis taken account to

primary pyrolysis and secondary cracking reactions with a total of 149 individual reactions. Calonaci et al. (2010) simulated biomass pyrolysis similar with Peters by using multistep kinetic model but with a limited number of reactions to discuss the gaseous products and tar species. Although such models offer high accuracy, they are often computationally intensive and require extensive experimental data making them less practical and incompatible for implementation in real-time applications or control system development. Therefore, this study aims to propose a simplified kinetic model that captures the essential reaction behaviour while ensuring computationally efficient, facilitating its application in process control and system optimization.

2. Materials and method

2.1 Biomass samples

The source of biomass is widely available in Japan. The biomass that was utilized in this study was selected as Hinoki (Japanese Cypress) from Tokyo, Japan. The important characteristics of Japanese Cypress for this research, such as proximate and ultimate values of the biomass, are summarized in the table below (Okada et al., 2008).

Table 1: Proximate and ultimate analysis of biomass feedstock

Proximate analysis	Value (wt.%)	Ultimate analysis, (dry ash free basis)	Value (wt.%)
Moisture Content (as determined basis)	10.78	C	51.4
Volatile Material (dry basis)	84	H	6.2
Fixed Carbon (dry basis)	16	N	0.2
Ash (dry basis)	0	O	42.2
		S	0

2.2 Modelling and simulation software

The biomass gasification simulation discussed in this paper was created based on Aspen Plus version 14 as shown in Figure 1. The gasification process was uncoupled into different parts based on the reaction mechanisms including pyrolysis, which occurs in the 'PYRO' reactor, tar cracking in 'TAREDC', and char reduction in both 'HETRO' and 'HOMO' reactors. These parts are linked with different types of reactors in the simulator. The process flowsheet and operating conditions were modified based on published paper by (Talero and Kansha, 2022).

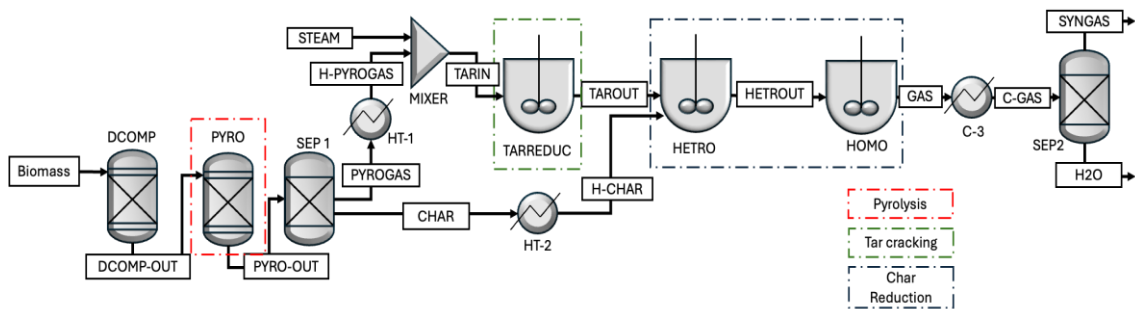


Figure 1: Process flowsheet of biomass gasification simulation







The development of the simulation model begins with specifying the stream class, selecting an appropriate property method, and inserting the required components from the database. Users must also identify both conventional and non-conventional components involved in the reaction. The next step is to define the process flowsheet by placing unit operation blocks and connecting them using material and energy streams. Finally, the input conditions for the streams and unit operation blocks are specified.

The descriptions of the blocks used in the simulation are shown in Table 2. Among all the streams in the flowsheet, only BIOMASS and STEAM are user-defined by specifying their inlet mass flow, temperature, and pressure. The stream class in this simulation is identified as MIXINC as the simulation involved solid and gas material. Peng-Robinson-Boston-Mathias (PB-RM) property was chosen in this simulation as this method is recommended for all temperatures and pressures, especially in gas processing, refinery, and petrochemical

applications. Reasonable results can be expected from these thermodynamic properties (Pala et al., 2017). Biomass and Char are defined as non-conventional components in the simulation process. The enthalpy and density models used for the non-conventional components were DCOALIGT and HCOALGEN.

A few assumptions were considered in this process modeling, including that the simulation was carried out under isothermal conditions, where temperature and pressure drop across the stream and inside the reactors were neglected. Additionally, the ash was assumed to be inert and was not considered in the reaction.

Table 2: Reactor block description used in the simulation

Default ID at Aspen Plus software		Assigned ID	Operating Condition	Description
RYield		DCOMP	100 kPa 650 °C	Yield reactor - converts biomass into conventional elements according to yield distribution data
RGIBBS		PYRO	100 kPa 650 °C	Gibbs reactor – simulates equilibrium pyrolysis product gas compositions by minimizing Gibbs free energy
SEP2		SEP1	100 kPa 650 °C	Separator – separates char from pyrolysis gases
		SEP2	100 kPa 25 °C	Separator – separates water from syngas
HEATER		HT-1	100 kPa 850 °C	To heat up the process stream to desire temperature
		HT-2	100 kPa 850 °C	To heat up the process stream to desire temperature
		C-3	100 kPa 25 °C	To cool down the process stream to desire temperature
Mixer		MIXER	100 kPa 850 °C	Mixer - mixes steam and gases
RCSTR		TARREDUC	100 kPa 850 °C	Continuous stirred tank reactor – tar reduction takes place
		HETRO	100 kPa 850 °C	Continuous stirred tank reactor – heterogenous gasification takes place
		HOMO	100 kPa 850 °C	Continuous stirred tank reactor – homogenous gasification takes place

2.3 Description of Aspen Plus flowsheet

The feed stream “BIOMASS” was dry basis biomass, specified as a non-conventional stream with the proximate and ultimate analysis values as shown in Table 1. The mass flow rate was set as 10 kg/h. The BIOMASS stream was connected to a yield reactor RYield block “DCOMP”. This decomposition reaction does not reflect any real reaction in real life. It is a virtual reaction step that decomposes biomass into its conventional components such as C, H₂, N₂, O₂, and H₂O. The output of the decomposition reactor was fed into a Gibbs reactor to simulate the pyrolysis reaction. The Gibbs reactor was chosen in this simulation as a simple and fast estimation of product components is needed. The reactor temperature was fixed at 650 °C, based on prior experimental results indicating that the pyrolysis products at this temperature closely approach thermodynamic equilibrium. The outlet stream “PYRO-OUT”, which contains C, CH₄, H₂, O₂, H₂O, CO, CO₂, and tar, was directed into the separator “SEP1” to separate the solid char and the pyrolysis gas. The pyrolysis gas is then mixed with the steam and fed into the CSTR reactor “TARREDUC” for tar reduction. The reactions that took place in this reactor were listed in Table 3 as R3. The tar produced (benzene, phenol, toluene, naphthalene) was turned into smaller hydrocarbons with the kinetic equations listed. Then, the gas produced is fed into the heterogeneous reactor “HETRO” to undergo a heterogeneous gasification process at 850 °C and 100 kPa, facilitated with reaction R1 followed by homogeneous reactor “HOMO” to undergo homogeneous gasification under the same temperature and pressure condition with reactor listed at R2 in Table 3. CSTR reactor is used to model tar cracking and char reduction in this simulation because it effectively captures the chemical reaction kinetics under the assumption of perfect mixing (Rabea et al., 2022). This ensures uniform reactant concentration and temperature throughout the reactor volume, making it suitable for simulating kinetically controlled, homogeneous and heterogeneous reactions. The CSTR configuration is particularly suitable for with complex and fast reactions where ideal mixing

can reasonably be assumed such as lab-scale gasification. Finally, the gas produced by the gasifier was sent into a separator to separate out the steam in the stream.

Table 3: List of reactions involved

No	Reaction	Kinetic	Reference
R1	$C + CO_2 \leftrightarrow 2CO$	$4.4Te^{\left(\frac{-1.62 \times 10^8}{RT}\right)} [CO_2]^{0.6}$	Yan et al. (2018)
	$C + H_2O \leftrightarrow CO + H_2$	$1.33Te^{\left(\frac{-1.47 \times 10^8}{RT}\right)} [H_2O]^{0.6}$	Yan et al. (2018)
R2	$CH_4 + H_2O \rightarrow CO + 3H_2$	$3.0 \times 10^5 e^{\left(\frac{1.25 \times 10^8}{RT}\right)} [CH_4]^1 [O_2]^1$	Beheshti et al. (2015)
	$CO + H_2O \rightarrow CO_2 + H_2$	$2.78 \times 10^6 e^{\left(\frac{-1.26 \times 10^7}{RT}\right)} \left([CO][H_2O] - \frac{[CO][H_2O]}{k_p(T)} \right)$ $k_p(T) = 0.0265e^{\left(\frac{4.55 \times 10^7}{RT}\right)}$	Yan et al. (2018)
R3	$C_6H_6 + 2H_2O \rightarrow 3C + 2CH_4 + 2CO$	$4.0 \times 10^{16} e^{\left(\frac{-4.43 \times 10^5}{RT}\right)} [C_6H_6]^{1.3} [H_2]^{-0.4} [H_2O]^{0.2}$	Peters et al. (2017)
	$C_7H_8 + H_2 \rightarrow C_6H_6 + CH_4$	$1.04 \times 10^{12} e^{\left(\frac{-2.47 \times 10^5}{RT}\right)} [C_7H_8]^1 [H_2]^{0.5}$	Peters et al. (2017)
	$C_6H_6O \rightarrow CO + 0.4C_{10}H_8 + 0.15C_6H_6 + 0.1CH_4 + 0.75H_2$	$10^7 e^{\left(\frac{10^5}{RT}\right)} [C_6H_6O]^1$	Peters et al. (2017)
	$C_{10}H_8 \rightarrow 9C + 0.16667C_6H_6 + 3.5H_2$	$3.4 \times 10^{14} e^{\left(\frac{3.5 \times 10^5}{RT}\right)} [C_{10}H_8]^{1.6} [H_2]^{-0.5}$	Peters et al. (2017)

3. Results and discussion

To validate the proposed simplified model for biomass gasification, the effects of gasifier temperature and steam-to-biomass (S/B) ratio were compared with values reported in the literatures. The influence of gasification temperature on syngas composition was evaluated over the range of 700 °C to 900 °C, in increments of 50 °C, at a constant S/B ratio of 1. Meanwhile, the effect of the S/B ratio was analyzed from 0.2 to 3.5, under a fixed gasification temperature of 850 °C. The deviation of simulation values from the literature data was calculated by calculating the root mean square error as Eq(1), y is the molar ratio, and n is the number of data set.

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (y_{exp,i} - y_{literature,i})^2}{n}} \quad (1)$$

3.1 Effect of gasification temperature

Figure 2a shows the effect of gasification temperature on the product gas composition at a S/B ratio of 0.8 for the Japanese Cypress. Based on the results, H_2 was the predominant gas produced, with a mole fraction of 0.53 at 700 °C. CO was the second most abundant at 0.24, followed by CO_2 at 0.15 and CH_4 at 0.05. As the temperature increased from 700 °C to 900 °C, the mole fraction of CO increased, while the mole fractions of H_2 and CO_2 decreased. This is consistent with previous simulation result by Babatabar and Saidi (2021). Furthermore, during these changes, the mole composition of CH_4 remained nearly constant (Inayat et al., 2010) and was the lowest number of gases produced (Talero and Kansha, 2022). Both trends can be observed in study carried out by Florin and Harris (2007). A similar trend can be observed from the study carried out by Pala et al. (2017), the amount of H_2 gas was the highest while the CH_4 was the lowest gas produced. However, from Pala's study, the production of H_2 was unaffected by increasing temperature, whereas CH_4 showed a slight decrease over time. At 900 °C, H_2 remained the predominant gas, although its mole fraction slightly decreased to 0.50. In contrast, CO showed an increasing trend, rising to 0.38. The concentrations of CO_2 and CH_4 remained relatively low, with mole fractions of 0.07 and 0.03, respectively, showing minimal change with temperature.

Reactions that took place in the heterogeneous gasification were the Boudouard reaction, water gas reaction, and steam reforming of methane. These reactions are endothermic reactions, favouring the forward reaction with increasing gasification temperature. This will increase the gas composition of H_2 and CO and decrease the

gas composition of CH_4 and CO_2 with temperature. The decrease of CO_2 gas composition with increasing gasification temperature may also be due to the exothermic reaction of the water gas shift reaction. The H_2 gas composition remains constant throughout the increment of temperature due to the generally low gas composition of CH_4 . The formation of H_2 gas is mainly dependent on the water gas shift reaction and the steam reforming of methane. The H_2/CO molar ratio decreases with increasing temperature as shown in Figure 2b. This is because the CO gas composition increases while the temperature increases, and H_2 remains constant. This proves that the Boudouard reaction was the dominant reaction in this steam-to-biomass ratio and gasification temperature range studied. Comparison of the simulated H_2/CO molar ratio and previous published work was done. The root mean square error of the simulated result and the study carried out by Babatabar and Saidi (2021) with S/B 0.5 is less than 0.34 %.

From this simulation result, 900 °C appeared to be the optimal temperature for the gasification process, as it produced the highest amount of CO and the lowest amount of CO_2 . CH_4 gas was not considered in this evaluation due to its minimal variation across the temperature range.

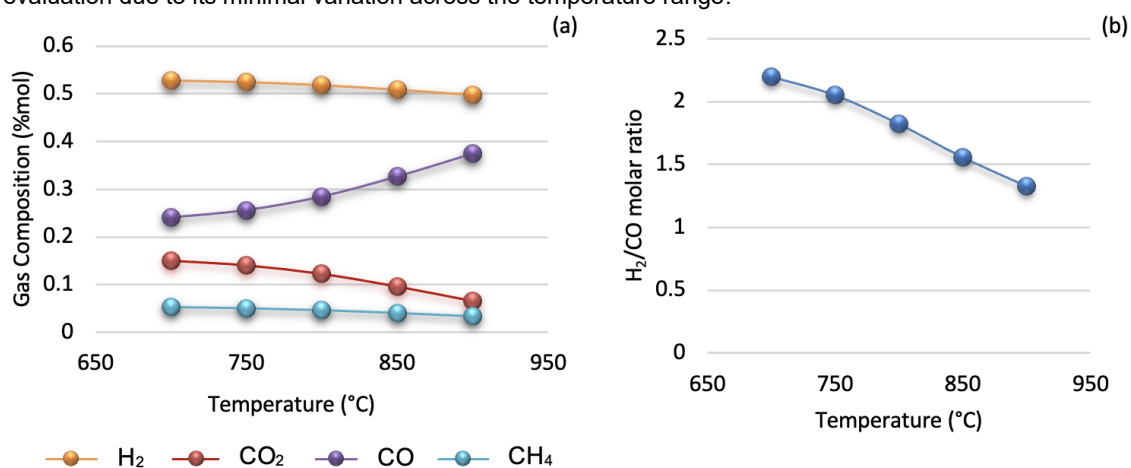


Figure 2: (a) Effect of the gasification temperature on the syngas composition; (b) Effect of temperature on H_2/CO molar ratio

3.2 Effect of steam to biomass (S/B) ratio

The effect of steam-to-biomass (S/B) ratio on the product gas composition was studied. The gasifier temperature and pressure were set to 850 °C and 100 kPa. Figure 3 shows the change in gas composition when varying the steam to biomass ratio. Increasing the steam-to-biomass ratio results in a marginal increase in the molar fraction of H_2 and a slight decrease in that of CH_4 .

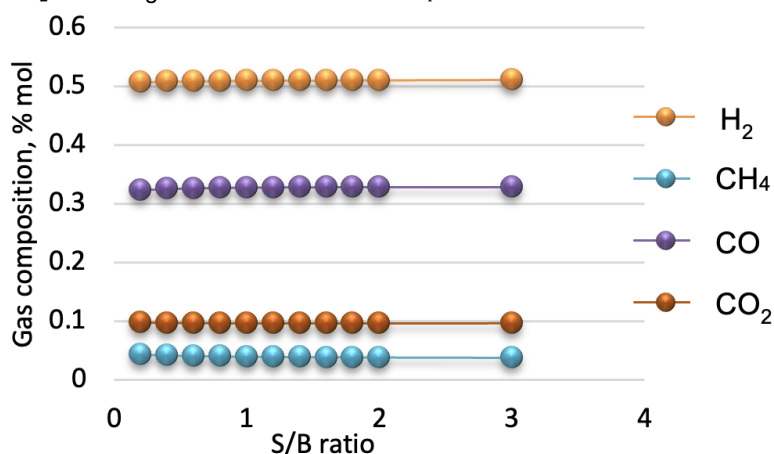


Figure 3: Effect of gasification temperature on S/B ratio

The molar fraction of the H_2 gas increases from 0.508 to 0.511 when increasing the steam to biomass ratio. Whereas the molar fraction of CH_4 gas shows a decrease from 0.0435 to 0.0373. Since steam is the only

gasification agent introduced in the whole gasification process, reactions such as methane reforming and water gas shift reactions are highly dependent on the steam feed rate. Therefore, at a higher steam-to-biomass ratio, the hydrogen mole composition will increase. A similar trend was also observed by Inayat et al. (2010).

4. Conclusions

A simple kinetic biomass gasification model is developed using the Aspen Plus simulator to discuss the syngas production during the steam gasification of Japanese Cypress. Each kinetic reaction captured in the model affects the biomass gasification process. In this study, results showed that 900 °C produced the highest CO and lowest CO₂ concentrations, indicating it as the optimal gasification temperature. This simulation model is compared with those presented in previous research to assess its relative performance and validity. It 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.

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