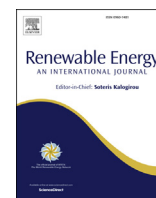


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Steam gasification of biomass with subsequent syngas adjustment using shift reaction for syngas production: An Aspen Plus model

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ABSTRACT

A simulation model of biomass gasification for syngas production with steam as gasifying agent and subsequent syngas adjustment has been developed using Aspen Plus. The developed model is based on Gibbs free energy minimization applying the restricted equilibrium method. The objective is to study the effect of important parameters such as gasification temperature, steam to biomass ratio and shift reaction temperature on hydrogen concentration, CO concentration, CO conversion, CO₂ conversion and H₂/CO ratio in the syngas. Simulations were performed for different biomass feedstocks to predict their syngas composition. The hydrogen and CO concentrations were altered such that the H₂/CO molar ratio in the syngas composition gets adjusted close to a value of 2.15 as required for FT synthesis by the shift reaction. The present model has been validated with experimental data from literature on steam biomass gasification conducted in a research scale fluidized bed gasifier. The product gas obtained from steam gasification of food wastes resulted in a composition with a H₂/CO molar ratio close to 2.15 which can be directly fed to a Fischer-Tropsch synthesis plant whereas remaining feedstocks requires a syngas adjustment either by WGS or RWGS reactions to achieve H₂/CO molar ratio close to 2.15.

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1. Introduction

Biomass is the most favorable renewable energy and CO₂ neutral source which can be a preferable choice for the replacement of conventional fossil fuels in the near future [1]. Biomass to liquid via Fischer-Tropsch synthesis (BTL-FT) is gaining increasing attention in recent years for the production of renewable fuels such as diesel, gasoline and jet fuel. Usually these fuels are clean and environmentally friendly and contain little or even no sulfur and other contaminant compounds, which can satisfy the upcoming stricter environmental regulations in both Europe and the US [2]. Diesel has gained support in Europe since the diesel engines of passenger cars have become competitive with that of gasoline, and currently, diesel represents half the fuel consumed by road transportation in the EU, while in the US it accounts for 22% of the road transportation. Therefore, the FT production method has received

attention for exploiting not only biomass but also natural gas reserves and coal, to produce liquid fuel hydrocarbons with high added-value [3]. The BTL process involves biomass gasification, syngas gas cleaning and adjustment, and Fischer-Tropsch synthesis. Fischer-Tropsch synthesis (FTS) uses syngas (synthesis gas) as a feed, which can be produced from biomass gasification, a thermochemical conversion process [4]. Gasification is a thermochemical process which converts carbonaceous materials into syngas. The gasification process can be split into four steps: biomass drying, pyrolysis, gasification and combustion. The syngas originating from biomass mainly consists of hydrogen and carbon monoxide, along with methane, carbon dioxide, water vapor, nitrogen and impurities such as tars, ammonia, hydrogen sulphide and hydrogen chloride. High quality syngas is often characterized by low N₂ content, high H₂ content, low tar levels and high heating value [5]. Steam gasification is often preferred as it improves the quality of the produced gas by increasing the hydrogen concentration. Besides, the steam gasification process has additional advantages such as maximizing the heating value, has advantageous residence time characteristics and efficient tar and char reduction [6].

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Among the three types of gasifiers; fixed bed, fluidized bed and entrained flow, the fluidized bed gasifiers are advantageous for biomass conversion due to the good heat and mass transfer between gas and solid phase and the high fuel flexibility and uniform and easier controllable temperature [7]. The H_2/CO ratio of the syngas produced from biomass gasification is between 1 and 2.2. The FTS with cobalt based catalysts in the BTL process requires a syngas as feed with a H_2/CO ratio of 2.15 for maximum liquid fuel production. Therefore, the H_2/CO ratio of the biomass generated syngas needs to be adjusted close to this ratio before it is fed to the FTS [8,9]. The adjustment can be done either by using forward shift or reverse shift reaction. It is also important that the biomass gasification matches the FTS requirements in terms of gas composition, levels of impurities and yields of the syngas to maximize the liquid fuel production. The biomass generated syngas quality and yield, on the other hand, depends on several factors such as the properties of the biomass, the gasifier type, the gasifier operating conditions, the gasifying agent and the complex chemical reactions which occur during gasification [10].

Aspen Plus is a simulation software tool which can be used for modeling biomass gasification processes and to predict the syngas composition for pre-defined biomass feedstock, gasification conditions and gasifying agent. Doherty et al. [5] developed a model in Aspen Plus for a fast internally circulating fluidized bed (FICFB) gasifier, which was successfully demonstrated at industrial scale (8 MW fuel input) in Güssing (Austria) since 2002 and validated against actual plant data. The model was based on Gibbs free energy minimization applying the restricted equilibrium method. They studied the impact of the operating parameters such as gasification temperature, biomass moisture, steam to biomass ratio, air-fuel ratio, and air and steam temperature and validated the model results against actual plant data and reported that predicted syngas composition, heating value and cold gas efficiency were in good agreement with published data. Begum et al. [11] developed an Aspen Plus model for an integrated fixed bed gasifier and predicted the steady-state performance of the model for different biomass feedstocks such as municipal solid wastes, wood wastes, green wastes and coffee bean husks. They studied the impact of operating variables, such as air-fuel ratio and gasifier temperature on syngas production. Sreejith et al. [12] developed an equilibrium model based on Gibbs free energy minimization for steam gasification of biomass using the Aspen Plus process simulator. They assumed that carbon is fully converted to product gases and no tar content is present in the gaseous product. They performed a sensitivity analysis for the product gas composition, its lower heating value, combustible gas yield, and energy efficiency and exergy efficiency on the gasification process variables including reactor temperature, pressure and steam to biomass ratio and validated the simulation results of the Aspen Plus model with published experimental results of steam gasification in a fluidized bed gasifier. They reported that model results slightly deviate from the experimental data and attributed this error to the tar formation which was not considered in the model. Nikoo and Mahinpey [13] developed a model for the biomass gasification in an atmospheric fluidized bed gasifier using the Aspen Plus simulation software. They validated the model against the experimental data from gasification of pine wood in a lab-scale fluidized bed gasifier. They studied the effect of operating variables, such as temperature, equivalence ratio (ER) defined as the ratio of actual biomass/air to the stoichiometry biomass/air, steam to biomass ratio and biomass average particle size on the product gas composition and carbon conversion efficiency. Im-orb et al. [14] developed a model for a biomass gasification combined with a Fischer Tropsch process using Aspen plus to perform a techno-economic analysis of the integrated process with rice straw feedstock for green fuel

production. They modelled oxygen supported gasification at 1000 °C, water gas shift at 150 °C to adjust H_2/CO ratio to 2.37, and a slurry phase FT reactor at 220 °C and 20 bar. They investigated the influence of changes in the FT off-gas recycle fraction on the performance of the syngas processor, the FT synthesis process as well as the economic feasibility of the entire BG-FT. They reported that the CO conversion and production rate of diesel from a FT synthesis unit increases whereas the electric power generation decreases when the FT reactor volume increases. According to their results an FT off-gas recirculation is less feasible than the once-through concept from an economic point of view. However, the authors did not compare different feed-stocks and the effect of these feed-stocks on syngas composition and operating conditions of the syngas adjustment through the shift reaction was also not subject of their work.

Though simulation models for biomass gasification process were developed using Aspen Plus, very few literature has been found on Aspen simulation models for biomass gasification and the subsequent syngas adjustment process using shift and reverse shift reactions. The purpose of this study is to develop an integrated model for steam gasification of biomass and subsequent syngas adjustment using shift reaction in Aspen Plus to predict the syngas composition from biomass. The model has been tested with different biomass feedstock compositions from literature such as coffee bean husks, green wastes, food wastes, Municipal Solid Wastes (MSWs), pine sawdust, wood residue and woodchips. The details of the modeling approaches taken to obtain a process simulation model for the gasification and WGS are presented in this work. The effect of operating parameters such as gasification temperature, steam to biomass ratio (S/B), shift temperature on the product gas compositions, CO conversion, CO_2 conversion and H_2/CO ratio has been studied. The predicted simulations results are validated with published experimental data of a research scale fluidized bed gasifier.

2. Biomass to biodiesel conversion process

Fig. 1 shows the steps involved in the production of diesel from biomass.

Firstly, biomass is gasified with steam as gasifying agent in a fluidized bed reactor. Product gas from the gasification mainly consists of H_2 , CO, CO_2 , CH_4 , H_2O , N_2 , char, ash and impurities such as tars, NH_3 , H_2S and HCl. Solids present in the product such as char, ash and tar are removed in a separator. At this point, the product gas composition may need to be adjusted to achieve a H_2/CO ratio close to 2.15 to make it suitable for feeding to a FT reactor. This is done by using a shift reactor. A separator is used to remove H_2O , CO_2 , H_2S , NH_3 and COS from the product gas, the remaining H_2 and CO mixture being the desired syngas. A detailed process description for the production of FT diesel from biomass can be found in Ref [3].

3. Aspen Plus modeling

The Aspen Plus flow-sheet for the biomass gasification and subsequent syngas adjustment using shift reactor is shown in Fig. 2. The development of a model in Aspen Plus involves the following steps:

Specification of the stream class, selection of the property method, specification of system components (from a data base) and identifying conventional and non-conventional components, defining the process flow-sheet (using unit operation blocks and connecting material and energy streams). Then the feed streams (flow-rate, composition and thermodynamic condition) and unit operation blocks (thermodynamic condition, chemical reactions, etc.) are specified.

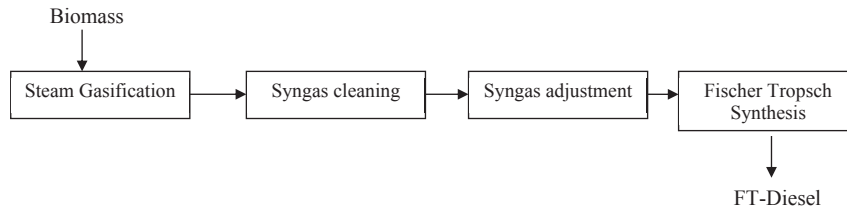


Fig. 1. Biomass to FT-Diesel production route.

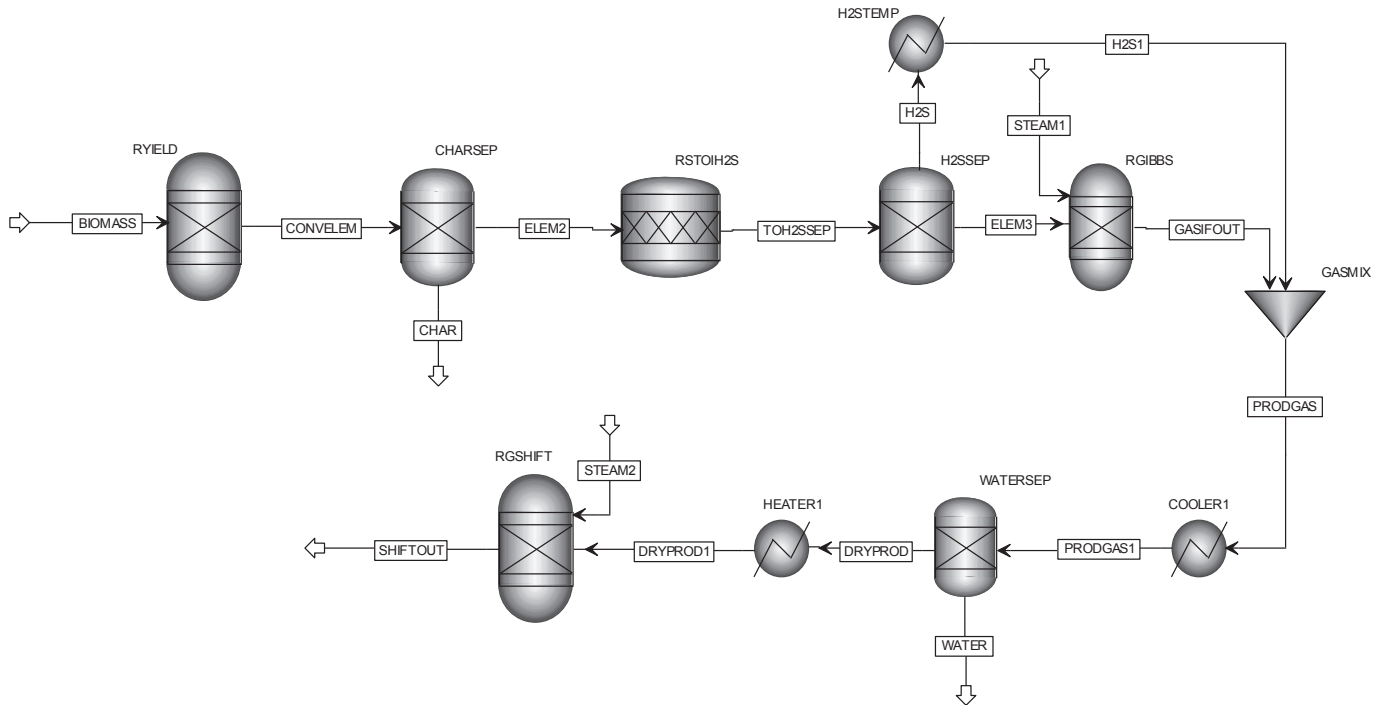


Fig. 2. Process Flowsheet for the Biomass Gasification and Shift reaction in Aspen Plus.

The following assumptions are made in this study to model the process:

1. Biomass feed rate is 1000 kg/hr and Steam is supplied at 1 bar and 150 °C
2. Process is steady state and isothermal
3. Pressure and temperature are uniform inside the gasifier
4. Operation at atmospheric pressure (~1 bar)
5. No heat and pressure losses occur in the gasifier
6. Tar formation is not considered and all fuel bond sulfur (S) is converted to H₂S [5].
7. No unconverted carbon is present in the product
8. Char only contains carbon and ash
9. Drying and pyrolysis are instantaneous [5].
10. All gases are ideal
11. The product stream contains H₂, CO, CO₂, CH₄, N₂, H₂O and H₂S only
12. The gases involved obey Peng-Robinson equation of state with Boston- Mathias (PR-BM) modification property method [5].

The types of biomass feed-stocks and their compositions used in this study are provided in Table 1.

It is well known that the real gasification process does not easily reach chemical equilibrium due to the short residence time in the

gasifier. Therefore, considerable deviations between predicted and experimental values of the syngas composition have been found when using the Gibbs equilibrium model [6]. Better agreement between the predicted and experimental syngas composition has been achieved by using the restricted equilibrium method to the Gibbs reactor model [5,16].

The present model is based on the RGibbs reactor model with the restricted chemical equilibrium. The restricted equilibrium is set by choosing the calculation option 'Restrict chemical equilibrium - specify temperature approach or reactions' to RGibbs block and individual reactions are defined with zero temperature approach specification. By specifying zero temperature approach to each reaction, RGibbs evaluates the chemical equilibrium constant for each reaction at reactor temperature thereby giving equilibrium gas composition. Biomass gasification is a complex process which involves several chemical reactions taking place inside the gasifier. Equations (1)–(8) listed in Table 2 are the chemical reactions considered in this work for the gasification process [5,11,12]. Nevertheless aspects of fluid dynamics, heat transfer limitations in the reactor and side reactions leading to tar formation and catalyst deactivation are not taken into consideration in the present model.

The Peng-Robinson equation of state with Boston- Mathias (PR-BM) modification has been chosen to calculate the thermodynamic properties of the conventional components in this model. PR-BM is recommended for gas processing, refinery and petrochemical

Table 1
Different Biomass Feedstocks and their Proximate and Ultimate Analysis.

Feedstock & composition	Coffee bean husks [11]	Green wastes [11]	Food wastes [11]	Municipal solid wastes [11]	Pine sawdust [13]	Wood chip [5]	Wood residue [15]
Moisture	10.1	48	29.3	48	8	20	5.01
Ultimate analysis (wt.%, dry)							
C	49.40	46.60	56.65	30.77	50.54	51.19	50.08
H	6.10	5.50	8.76	4.62	7.08	6.08	6.70
O	41.20	38.61	23.54	17.30	41.11	41.30	42.51
N	0.70	0.71	3.95	0.77	0.15	0.20	0.16
S	0.07	0.18	0.19	0.39	0.57	0.02	0.20
Cl	0.03	—	—	—	—	0.05	—
Ash	2.50	8.40	6.91	46.15	0.55	1.16	0.36
Proximate analysis (wt.%, dry)							
Volatile matter	14.30	72.00	72.41	46.15	82.29	80.00	81.81
Fixed carbon	83.20	19.60	20.68	7.70	17.16	18.84	17.83
Ash	2.50	8.40	6.91	46.15	0.55	1.16	0.36

Note: The values shown in the above table are as to be fed into the Aspen Plus model.

Table 2
Chemical reactions involved in the process.

Reaction number	Reaction scheme	Reaction name	Heat of reaction ΔH (KJ/mol)
1	$C + O_2 \rightarrow CO_2$	Carbon combustion	-393.0
2	$C + 0.5O_2 \rightarrow CO$	Carbon partial oxidation	-112.0
3	$C + CO_2 \rightarrow 2CO$	Boudouard reaction	+172.0
4	$C + H_2O \rightarrow CO + H_2$	Water gas reaction	+131.0
5	$CO + H_2O \rightarrow CO_2 + H_2$	Water gas shift reaction	-41.0
6	$C + 2H_2 \rightarrow CH_4$	Methanation of carbon	-74.0
7	$H_2 + 0.5O_2 \rightarrow H_2O$	Hydrogen partial combustion	-242.0
8	$CH_4 + H_2O \rightarrow CO + 3H_2$	Steam reforming of methane	+206.0
9	$H_2 + S \rightarrow H_2S$	H_2S formation	-20.2

applications such as gas plants, crude oil conversion and ethylene plants. This method is used for nonpolar or mildly polar mixtures like hydrocarbons and light gases such as CO_2 , H_2S and H_2 . Using PR-BM, reasonable results can be expected at all temperatures and pressures. This property method is consistent in the critical region. To describe the water-gas shift reactor an RGibbs reactor model has been applied. A validation of the WGS reactor model was not performed, because the reaction system is simple and WGS reactors usually achieve equilibrium especially at the relatively high temperatures applied.

3.1. Description of Aspen Plus flow-sheet

The process flow-sheet of the biomass gasification and shift reaction is shown in Fig. 2. The feed BIOMASS was specified as a non-conventional stream and the mass flow rate of 1000 kg/hr was chosen as basis. Under component attributes of the stream BIOMASS, the ultimate and proximate analyses of the biomass feedstock were entered. The BIOMASS stream goes to yield reactor RYIELD block where pyrolysis occurs to form conventional components such as Carbon (C), H_2 , O_2 , N_2 , S, steam (H_2O) and Ash. This was done by specifying the yields distribution to the RYIELD reactor block according to the ultimate analysis of the feedstock. Yield distribution represents the yields of each component generated during pyrolysis. This determines the mass flow of each component in the RYIELD block outlet stream CONVELEM. Ash was selected as non-conventional component and 100% of ash was set for the ultimate and proximate analysis under component attributes of Ash. The outlet stream CONVELEM from the RYIELD block goes to the separator column, CHARSEP. This separator column CHARSEP separates out char (fixed carbon) and ash as stream CHAR and remaining components such as C, H_2 , O_2 , N_2 , S and H_2O as stream ELEM2. The char split fraction is set based on the fixed carbon and ash split fraction is set to 1. The stream ELEM2 containing C, H_2 , O_2 , N_2 , S and H_2O enters the stoichiometric reactor RSTOIH2S block, where all the sulfur present in the feedstock is converted to H_2S

according to equation (9). This is done by specifying fractional conversion of 100% for sulfur. Due to the low contents of sulfur in the fuel, inaccuracies because of the assumption that all sulfur converts to H_2S are negligible [17]. The outlet stream from the RSTOIH2S reactor, TOH2SSEP containing C, H_2 , O_2 , N_2 , H_2O and H_2S is directed to the separator column H2SSEP, where H_2S gas is separated out as stream H2S. The stream ELEM3 from the separator column H2SSEP is the main fuel stream consisting of C, H_2 , O_2 , N_2 and H_2O . The main fuel stream ELEM3 goes to the gasification reactor RGIBBS where the gasification process takes place. The gasifying agent steam is added to the RGIBBS reactor as stream STEAM1.

In the block 'RGIBBS' reactor, gasification temperature is varied between 750 and 950 °C and the stream 'STEAM1' mass flow rate is varied depending on the steam to biomass (S/B) ratio between 0.2 and 1. The gasification reactions Eq. (1)–(8) are specified to the RGIBBS block. The outlet stream GASIFOUT from the block RGIBBS reactor contains H_2 , CO, CO_2 , N_2 , H_2O and CH_4 . The stream 'H2S', containing hydrogen sulphide, is raised to gasification temperature using the heater block 'H2STEMP' and comes out as stream 'H2S1'. The stream 'H2S1' and the outlet stream 'GASIFOUT' from the 'RGIBBS' reactor are mixed using the mixer block 'GASMIX' and the exit stream, containing hydrogen, nitrogen, steam, methane, carbon monoxide, carbon dioxide and hydrogen sulphide comes out as 'PRODGAS'. The stream PRODGAS represents the product gas from the gasifier. The stream 'PRODGAS' goes to heater block 'COOLER1'. The temperature of the heater block COOLER1 is set to 25 °C. The outlet stream 'PRODGAS1' from COOLER1 is fed to the separator WATERSEP, where water is separated out from the stream PRODGAS1. The degree of water removal is obviously determined by the condensation temperature adjusted. The stream containing H_2 , N_2 , CH_4 , CO, CO_2 and H_2S is represented as DRYPROD. The stream DRYPROD goes to the heater block HEATER1, which is maintained at 150 °C and comes out as the stream DRYPROD1. The stream DRYPROD1 is sent to block RGSIFT reactor, where shift reaction takes place according to Eq. (5). The shift reactor

Table 3
Reactor block description used in the simulation.

Block ID	Aspen Plus name	Description
RYIELD	RYield	Yield reactor – converts biomass in to conventional elements according to yield distribution data
CHARSEP	Sep	Separator – separates char and ash
RSTOIH2S	RStoic	Stoichiometric reactor; models the reactor with specified reaction extent or conversion. Useful where reaction kinetics are unknown or unimportant and stoichiometry and extent of reaction are known
H2SEP	Sep	Separator – separates hydrogen sulfide
RGIBBS	RGibbs	Equilibrium reactor; models single phase chemical equilibrium or simultaneous phase and chemical equilibrium by minimizing Gibbs free energy. Useful when temperature and pressure are known and reaction stoichiometry is unknown
H2STEMP	Heater	Heater – used to heat H ₂ S stream
GASMIX	Mixer	Stream mixer – mixes the H ₂ S with product gas
COOLER1	Heater	Cooler – cools down the product gas temperature to 25 °C
RGSHIFT	RGibbs	Equilibrium reactor; models single phase chemical equilibrium or simultaneous phase and chemical equilibrium by minimizing Gibbs free energy. Useful when temperature and pressure are known and reaction stoichiometry is unknown
WATERSEP	Sep	Separator – separates water from the produced gas
HEATER1	Heater	Heater – preheats the dry product gas to 150 °C

temperature and feed composition is manipulated in such a way that the H₂ and CO concentrations in the stream DRYPROD1 gets adjusted to result in H₂/CO molar ratio close to 2.15 in the shift reactor outlet stream SHIFTOUT. Either water is removed by condensation as described above or even added through addition of steam (STEAM2). Nitrogen, methane and hydrogen sulfide present in the stream 'DRYPROD1' are kept as inert in the 'RGSHIFT' block. The WGS reaction eq. (5) is specified to the block RGSHIFT. The shift reactor is considered as sour shift reactor because hydrogen sulphide is also present in the inlet stream 'DRYPROD1'.

Seventeen material streams were used in the flow-sheet. Among these material streams, only BIOMASS, STEAM1 and STEAM2 are user defined streams. A description of the blocks used in the flow-sheet is shown in Table 3.

4. Results and discussion:

4.1. Model validation

In order to validate the present model, a comparison has been made between the predicted gas composition obtained through gasification from the developed simulation model with the

experimental data published by Fremaux et al. [15]. They conducted steam gasification of wood residue as biomass feedstock in a research scale fluidized bed gasifier. Characteristics of wood residue used in their work are shown in Table 1. They studied the effect of gasification temperature at 700 °C, 800 °C and 900 °C and the steam to biomass ratio between 0.5 and 1. For comparison, the predicted results were obtained by running the model for wood residue at gasification temperatures of 700 °C and 900 °C, and steam to biomass ratios between 0.5 and 1.

Fig. 3(a) shows the comparison of the product gas composition between the present model and experimental data at a gasification temperature of 700 °C. It can be observed that the present model shows similar trends as they were found in the experiments. The model predicted higher hydrogen concentrations than the experimental data. The reason for this could be, that the model does not consider the formation of tar and higher hydrocarbons. Similar argument was made by Liao et al. [16] while validating their model results with the pilot scale dual fluidized bed gasifier in their work. Fremaux et al. [15] reported high tar concentrations at a gasification temperature of 700 °C and the decrease in tar concentration with increasing steam to biomass ratio. Also the formation of methane is underestimated by the model, which has a significant impact only

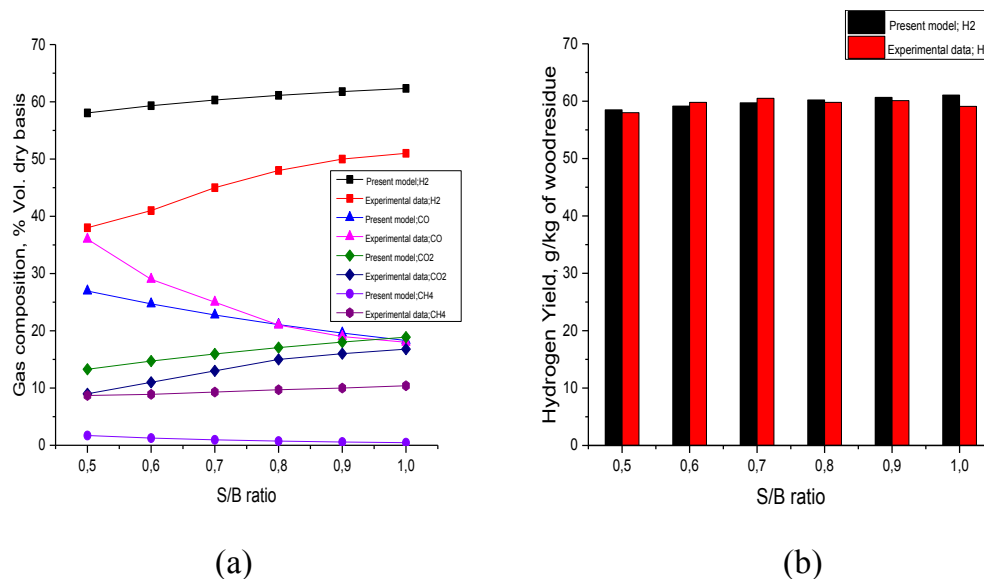


Fig. 3. (a) Effect of the S/B ratio on the product gas composition of the gasifier at a gasification temperature of 700 °C; (b) Effect of S/B ratio on the hydrogen yield of the gasifier at a gasification temperature of 900 °C; Experimental data from Fremaux et al. [15].

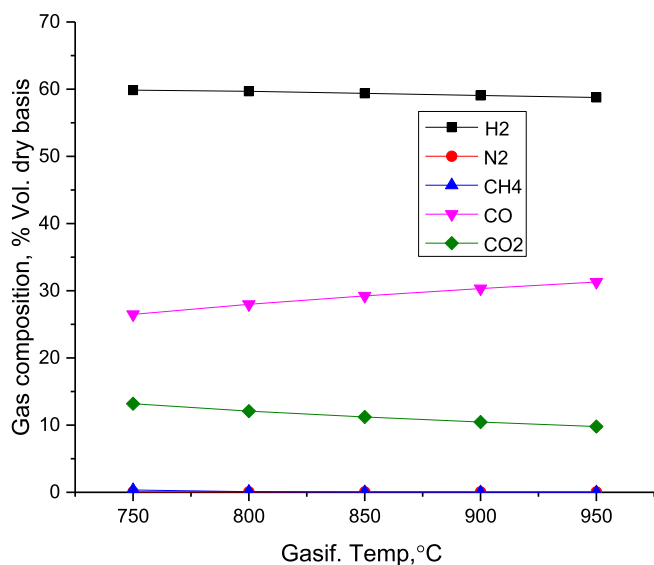


Fig. 4. Effect of the gasification temperature on the product gas composition of the gasifier at a S/B ratio of 0.6 for wood residue.

at low gasifier temperatures as indicated above. Fig. 3(b) shows the comparison of predicted hydrogen yield with that of experimental data at a gasification temperature of 900 °C. It can be seen that the predicted hydrogen yields are in good agreement with the experimental yields. Fremaux et al. [15] reported that the higher hydrogen yields were due to the reduction in tar formation with increase in temperature and recommended a gasification temperature of 900 °C as optimum value.

Using the validated model, the effect of operating variables such as gasification temperature (Gasif. Temp), steam to biomass ratio (S/B), shift temperature (Shift Temp) on gas composition, CO conversion, CO₂ conversion and H₂/CO molar ratio has been investigated. The gasification temperature has been varied between 750 and 950 °C; the steam to biomass ratio has been varied between 0.2 and 1 and the shift temperature between 250 and 900 °C. During the parameter analysis, only one input parameter is varied while other parameters are kept constant.

4.2. Effect of gasification temperature

The product gas composition was obtained for the feed-stocks shown in Table 1 by varying the gasification temperature

between 750 and 950 °C and S/B ratio between 0.2 and 1. Fig. 4 shows the effect of the gasification temperature on the product gas composition at a S/B ratio of 0.6 for the wood residue.

It can be observed that the concentration of CO increases with increase in temperature whereas the concentrations of CO₂ and CH₄ decrease with increasing temperature. The concentration of hydrogen remains almost the same for all gasification temperatures. Similar trends were reported in Refs. [18,19]. The same trends were observed for the remaining feed-stocks (not shown here).

As represented in Table 2, the Boudouard reaction, water gas reaction and steam methane reforming are endothermic reactions favoring their forward reaction with increasing gasification temperature. This will result in an increase of the concentrations of H₂ and CO with temperature and a decrease of the methane and CO₂ concentrations. Methanation is an exothermic reaction which favors the backward reaction with increasing temperature and therefore also decreases methane formation. The decreasing CH₄ formation is however mostly determined by the effect of steam methane reforming, which is dominant at high temperatures. The decreasing CO₂ concentration with increasing gasification temperature could be due to the effect of the Boudouard reaction coupled with the reversible WGS reaction. Due to the generally low concentration of methane, the hydrogen formation is mainly determined by the water gas and water-gas shift reactions which resulted in an almost constant hydrogen concentration with increasing gasification temperature.

Fig. 5 shows the effect of gasification temperature on H₂/CO molar ratio in the product gas composition at a S/B ratio of 0.6.

It can be seen that the H₂/CO ratio decreases with increasing biomass gasification temperature. The reason is that the increasing gasification temperature resulted in increasing CO concentration whereas the H₂ concentration remained almost constant. This indicates that the Boudouard reaction was the dominating reaction over the water gas reaction in the gasification temperature range studied.

4.3. Effect of steam to biomass (S/B) ratio

Fig. 6 shows the effect of the S/B ratio on the product gas composition at a gasification temperature of 900 °C for the wood residue. It can be observed that the concentration of H₂ and CO₂ increases with increasing S/B ratio whereas the concentrations of CO and CH₄ decrease with S/B ratio. Similar trends were reported in Refs. [18,19]. The same trends were observed for the remaining feed-stocks (not shown here).

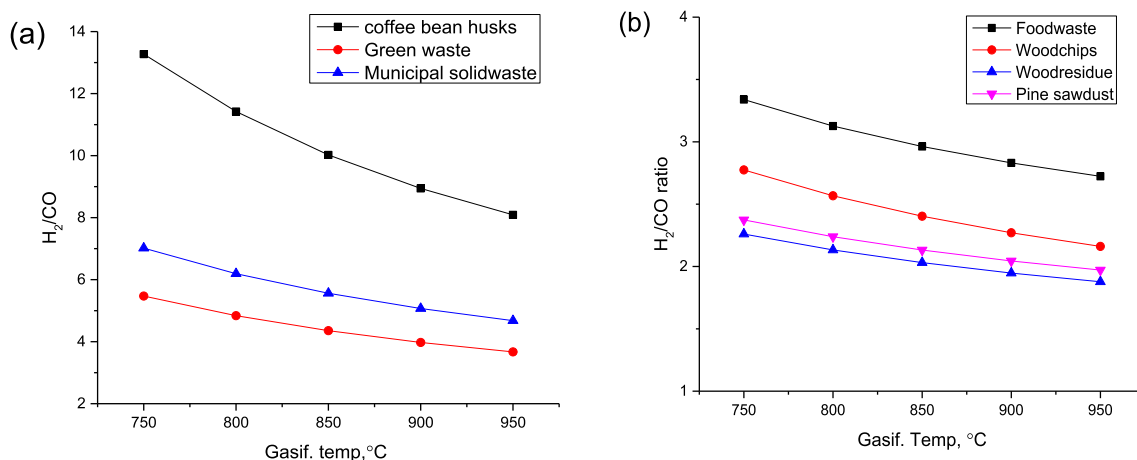


Fig. 5. Effect of the gasification temperature on H₂/CO molar ratio in the product gas composition of the gasifier at S/B ratio of 0.6 for different feedstock.

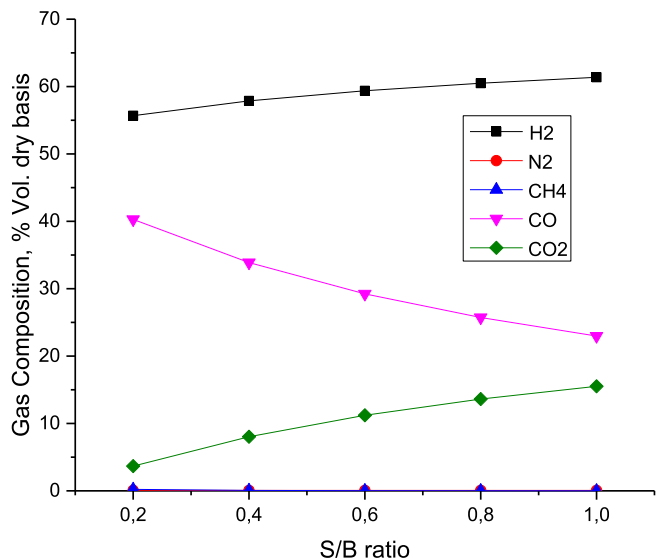


Fig. 6. Effect of the S/B ratio on the product gas composition of the gasifier at a gasification temperature of 900 C for wood residue.

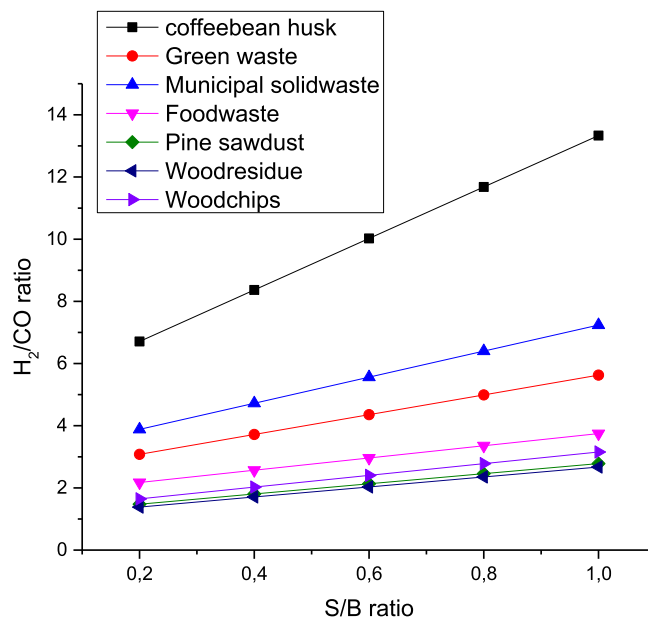


Fig. 7. Effect of the S/B ratio on H_2/CO ratio in the product gas composition of the gasifier at a gasification temperature of 900 °C.

Table 4

Gas compositions of the gasifier product as determined by the simulation for different feedstock at a gasification temperature of 900 C and S/B ratio of 0.2

Feedstock	H_2	N_2	CH_4	CO	CO_2	H_2S , ppmV	H_2/CO
Wood residue	55.71	0.07	0.08	40.76	3.31	800.69	1.37
Wood chips	56.59	0.09	0.02	35.40	7.90	78.11	1.6
Pine sawdust	57.09	0.07	0.07	39.19	3.36	2173.90	1.46
Municipal solid wastes	65.87	0.39	0.002	18.26	15.31	1726.37	3.61
Food wastes	64.39	1.29	0.04	30.22	3.99	542.61	2.13
Green wastes	60.63	0.32	0.0019	21.18	17.79	701.45	2.86
Coffee bean husks	68.64	1.09	0.0003	11.29	18.88	953.18	6.08

Since more steam is added to the feed with increasing S/B ratio, it enhances the water gas and steam methane reforming reactions which result in an increase of H_2 and CO concentrations. However, the CO concentration decreases with increasing S/B ratio. This is due to the WGS reaction which reduces CO concentration reacting with steam and increasing H_2 and CO_2 concentrations. It can be observed that the effect of S/B ratio on the hydrogen concentration was weak. The weak effect of S/B ratio on the hydrogen concentration was also reported in Ref. [20]. Therefore, it is advantageous to feed only a low amount of steam because the production of steam is an energy intensive process [12].

Fig. 7 shows the effect of the S/B ratio on the H_2/CO ratio in the product gas composition at a gasification temperature of 900 °C. It can be observed that the H_2/CO ratio increases with increasing S/B ratio. The reason solely originates from the effect of the WGS reaction taking place in the gasifier favoring more hydrogen formation accompanied with a reduction of the CO concentration owing to the presence of a higher amount of steam.

The simulated gas compositions obtained at a gasification temperature of 900 °C and S/B ratio of 0.2 from the gasifier for the feedstocks studied in this work was shown in Table 4. It can be seen that hydrogen content and H_2/CO ratio was highest for coffee bean husks and lowest for the wood residue. An effect of the moisture content on the gas compositions could not be derived.

From Table 4, it is seen that the H_2/CO molar ratio in the product gas composition resulting from the steam gasification of food wastes is close to 2.15, which can be fed directly to FT synthesis

without requiring syngas adjustment whereas the product gas compositions obtained from the steam gasification of the remaining feed-stocks needs syngas adjustment before feeding to the FT synthesis. The syngas adjustment can be done through forward

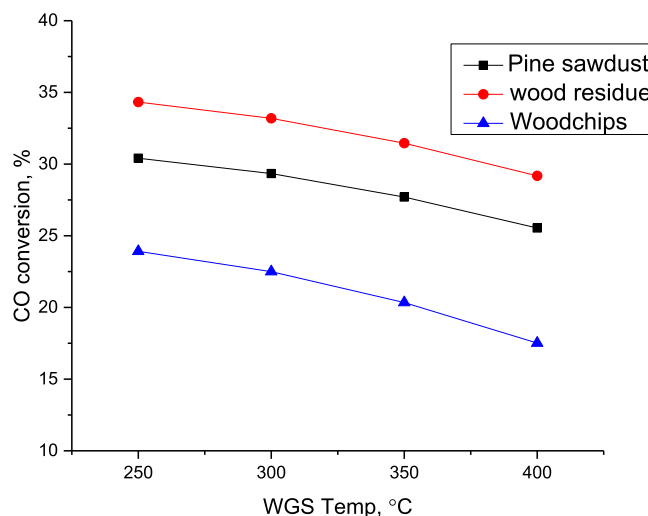


Fig. 8. Effect of the WGS temperature on the CO conversion at a gasification temperature of 900 °C and S/B ratio of 0.2.

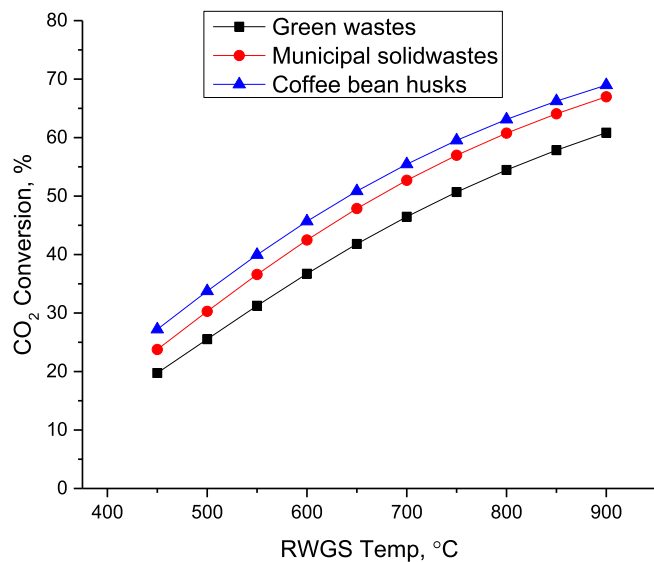


Fig. 9. Effect of the RWGS temperature on the CO₂ conversion at a gasification temperature of 900 °C and S/B ratio of 0.2.

concentrations were in the range of 50–600 ppmV [21] for syngas determined experimentally from different biomass feed-stocks. It should be noted that biomass-derived syngas also contains small amounts of COS along with H₂S, which was not considered in the model assuming that the all fuel based sulfur is converted to H₂S.

4.4. Effect of shift reaction temperature

The WGS reaction (Eq. (5)) is an exothermic reversible reaction which favours formation of reactants at higher temperatures. WGS reaction is favoured in the temperature range of 250–400 °C whereas RWGS is favoured at higher temperatures. The forward shift reaction is applied to the product gas obtained from steam gasification of wood residue, woodchips and pine sawdust whereas reverse shift reaction is applied to the product gas obtained from steam gasification of municipal solid wastes, green wastes and coffee bean husks.

Fig. 8 shows the effect of the WGS temperature on CO conversion. It is obvious from the thermodynamic equilibrium that the CO conversion decreases with increasing WGS temperature.

Fig. 9 shows the effect of the RWGS temperature on CO₂ conversion. It can be seen that the CO₂ conversion increases with

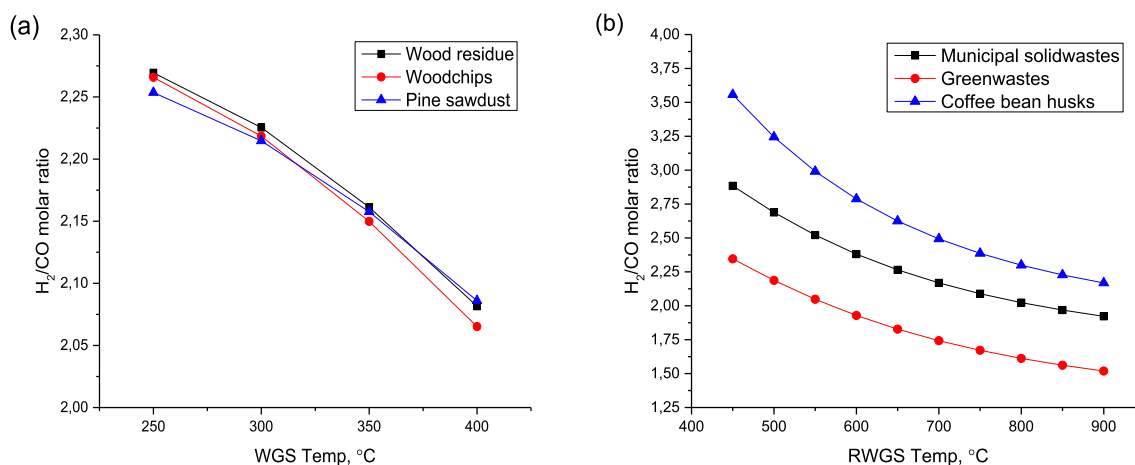


Fig. 10. Effect of the WGS and RWGS temperature on the H₂/CO molar ratio of the shift reactor outlet composition at a gasification temperature of 900 C and S/B ratio of 0.2.

shift or reverse shift reactions depending on the requirement to increase or decrease the H₂/CO molar ratio. The predicted H₂S concentrations are in the range of 78–2174 ppmV whereas H₂S

increasing RWGS temperature in the range of 450–900 °C [22].

Fig. 10 shows the effect of shift temperature on the H₂/CO ratio of the shift reactor outlet composition at a gasification temperature

Table 5

Optimum parameter conditions and corresponding product gas compositions obtained after syngas adjustment for the feedstocks for a gasification temperature of 900 °C and S/B ratio of 0.2

Feed-stock →	Wood residue	Woodchips	Pine sawdust	Municipal solid wastes	Green wastes	Coffee bean husks
Result ↓						
Shift Temperature, °C	350	350	350	700	500	900
(Steam/CO) _{inlet}	0.28	0.20	0.25	5.47E-05	4.72E-05	8.86E-05
(CO ₂ /H ₂) _{inlet}	0.06	0.14	0.06	0.24	0.31	0.27
H ₂ , dry vol%	59.68	59.80	60.39	62.78	58.78	63.56
N ₂ , dry vol%	0.07	0.08	0.06	0.43	0.33	1.27
CH ₄ , dry vol%	0.20	0.06	0.19	0.01	0.01	0.002
CO, dry vol%	27.61	27.48	27.99	28.95	26.87	29.32
CO ₂ , dry vol%	12.37	13.29	11.17	7.65	13.94	5.74
H ₂ O, vol%	1.25	1.33	1.12	9.22	5.55	13.54
CO Conversion, %	31.46	20.34	27.70	—	—	—
CO ₂ Conversion, %	—	—	—	52.69	25.52	68.98
H ₂ /CO ratio	2.16	2.15	2.16	2.17	2.19	2.17

of 900 °C and a S/B ratio of 0.2. It can be seen that H₂/CO decreases with increasing WGS and RWGS reaction temperature. This is explained by the concomitant decrease in CO conversion with increasing WGS temperature and increase in CO₂ conversion with increasing RWGS temperature.

The parametric conditions and corresponding gas compositions of the feed-stocks which resulted in H₂/CO molar ratio close to 2.15 after syngas adjustment by WGS and RWGS reactions at a gasification temperature of 900 °C and S/B ratio of 0.2 studied in this work are shown in Table 5.

5. Conclusion

An Aspen Plus model has been developed for the steam gasification of biomass and syngas adjustment processes using the shift reactions. The model is based on the Gibbs free minimization of energy applying the restricted equilibrium method and the temperature approach has been specified for each reaction involved in the gasification process. The Peng–Robinson equation of state with Boston–Mathias (PR-BM) modification has been chosen as base property method. The effects of operating parameters such as gasification temperature, steam to biomass ratio and shift temperature on the gas composition, CO conversion, CO₂ conversion and H₂/CO molar ratio has been investigated. Different biomass feed-stocks such as coffee bean husks, green wastes, food wastes, municipal solid wastes (MSWs), pine sawdust, wood residue and woodchips were investigated to predict their syngas composition. The results indicate that the hydrogen content almost remains constant with increasing gasification temperature whereas it increases with increasing steam to biomass ratio. As expected, the hydrogen and CO concentrations are altered such that the H₂/CO molar ratio gets adjusted by WGS and RWGS reaction. As expected from the thermodynamic equilibrium, the CO conversion decreases with increasing water gas shift temperature between 250 and 400 °C. The CO₂ conversion increases with increasing reverse water gas shift temperature between 450 and 900 °C. The H₂/CO molar ratio was found to decrease with increasing gasification temperature whereas it increases with increasing steam to biomass ratio. The validation of the model with experimental data from a gasifier operated at a lower reaction temperature as applied for the current calculations revealed basic agreement, however, the methane formation was underestimated and consequently the hydrogen content overestimated. At higher operating conditions, the predicted hydrogen content from the simulation model was found to be in good agreement with experimental data. Among the feedstock employed with this model, product gas obtained from steam gasification of food wastes can be directly fed to FT synthesis without syngas adjustment. Product gas obtained from steam gasification of wood residue, woodchips and pine sawdust requires syngas adjustment by WGS reaction whereas product gas obtained from steam gasification of municipal solid wastes, green wastes and coffee bean husks requires syngas adjustment by RWGS reaction to result in H₂/CO molar ratio close to 2.15 desirable to be fed to FT synthesis.

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