

Simulation of Syngas Production via Pyrolysis-oil Gasification – Impacts of Operating Conditions on Syngas Properties

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A model for syngas production from pyrolysis oil gasification was developed, validated, and used in this work to predict the effect of operating conditions on syngas properties. The model consists of a process line that includes units for pyrolysis-oil drying, decomposition, combustion, and gasification processes. The model was validated using experimental data from the literature, showing a good agreement between the results and the reference method. Syngas potential applications were assumed, e.g., for direct use in fuel cells and fuel production. Sensitivity analysis was carried out to evaluate the impacts of gasifying agent, temperature, and the oil moisture content on syngas composition, lower heating value (LHV), and H₂:CO molar ratio. For fuel cells applications, gasifying with O₂ and air lead to a substantial decrease in syngas LHV. The syngas should be produced at a high temperature. The moisture content in pyrolysis-oil also should be minimized. For fuel production applications, partial O₂ can be used to adjust the H₂:CO molar ratio. The syngas should be produced at an appropriate temperature around 1000°C. The moisture content in pyrolysis oil should also be selected at 40%.

Keywords: Renewable resources; Syngas composition; H₂:CO molar ratio; Lower heating value; Aspen Plus model;

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INTRODUCTION

The annual global energy consumption is approximately 14000 Mtoe (million tons of oil equivalent), 80% to 85% of which is supplied by fossil fuels (Mirandola and Lorenzini 2016). The steady increase in global energy consumption has led to an alarming rise in greenhouse gases (GHG) emissions such as CO₂, NO_x, and SO_x pollutants into the environment. The GHG emissions from fossil fuels have a dominant influence on increasing atmospheric CO₂ concentration that translates into rising global temperatures and sea levels. Considering the rapidly increasing global energy demand and the growing concerns about the environmental challenges, renewable and sustainable energy (e.g., solar, wind, and biomass) is a key solution to the energy crisis. Biofuels are promising alternatives to fossil fuels. As the biofuels are derived from renewable energy sources, the CO₂ emissions caused by their combustion are reabsorbed by newly grown biomass (McKendry 2002).

Pyrolysis-oil, also called bio-oil, is a complex blend of numerous oxygenated hydrocarbons produced from lignocellulosic biomass by fast pyrolysis process in the

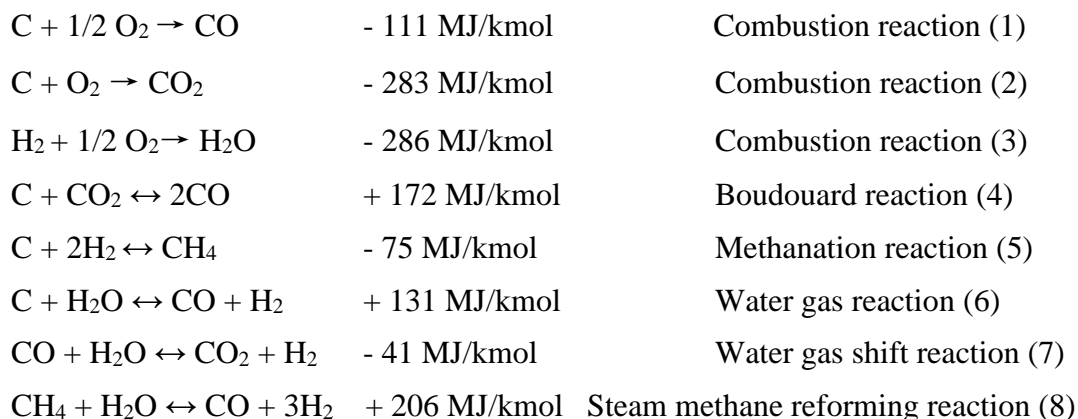
temperature range from 400 °C to 600 °C in the absence of oxygen (Alvarez *et al.* 2014). This liquid contains carboxylic acids, alcohols, aldehydes, ketones, esters, furans, and aromatics (Staš *et al.* 2014). The water content of the pyrolysis-oil generally ranges from 15 wt% to 25 wt% (Bridgwater and Cottam 1992; Radlein 1999). Up to 70 wt% of the original dry biomass can be converted into pyrolysis oil (Chang *et al.* 2013). The composition of pyrolysis-oil depends on such factors as the type of biomass feedstock, alkali content, reactor type, pyrolysis temperature, residence time, efficiency of char removal, *etc.* (Brown *et al.* 2001; Huber *et al.* 2006; Demirbas 2007).

Pyrolysis-oil offers several advantages over primary biomass sources, which means that there is potential to expand the scope of biomass feedstock applications. The volumetric energy density is increased about five times over that of “bulk” biomass, making transportation economically more attractive, especially over long distances (Van Rossum 2009). When large-scale remote biomass collection is considered, pyrolysis-oil can first be produced locally and then transported to a central processing area to synthesize liquid hydrocarbons (Van Rossum 2007). Secondly, the pyrolysis-oil being a liquid makes its storage, transportation, processing, and pressurization easier. During storage, the pyrolysis oil becomes more viscous due to chemical and physical changes: many polymerization reactions occur, and volatiles are emitted with aging. Thus, the pyrolysis-oil can also be stored in tanks at low temperature that have good resistance against degradation and cannot be ignited at ambient temperature (Oasmaa and Meier 2005). Finally, pyrolysis-oil contains only a small amount of sulfur, nitrogen, and ash. Therefore, its combustion produces less harmful gas emissions such as nitrogen oxides (NO_x) and sulfur dioxide (SO₂), compared to conventional fossil fuels (Van Rossum 2009). Furthermore, as the pyrolysis-oil is produced through a low-temperature process, minerals and metals remain in the solid char residue.

Pyrolysis-oil can be upgraded to liquid fuels and is considered as an energy carrier. However, the drawbacks of the oil are numerous and limit its applications. The use of pyrolysis-oil offers some challenges due to its properties, such as the low lower heating value (LHV), high oxygen content, volatility, high viscosity, acidity, chemical instability, and incompatibility with respect to standard petroleum fuels (Oasmas and Czernik 1999). Therefore, research is being conducted to upgrade pyrolysis-oil and enlarge its scope of applications. For example, Elliott *et al.* (2009) investigated catalytic hydrocarbons as a way to convert pyrolysis oil into hydrocarbons, alkanes, and aromatics. Pyrolysis oil was being used to produce syngas through gasification (Rossum *et al.* 2009; Postma *et al.* 2016). Bleeker *et al.* (2007) suggested using pyrolysis-oil to produce pure hydrogen. The research showed that hydrogen can be produced through the oxidation of pyrolysis-oil with a yield of 0.84 Nm³/kg dry pyrolysis oil (LHV H₂/LHV oil = 0.4).

During gasification process, several thermochemical reactions take place at various temperature ranges: Drying (>150 °C), decomposition (250 °C to 700 °C), combustion (700 °C to 1500 °C), and gasification (800 °C to 1000 °C). During drying stage, the moisture content is reduced from pyrolysis-oil. The decomposition stage is initiated at about 250 °C when the labile bonds between the aromatic clusters are cleaved, generating light molecular weight fragments. This stage generates gaseous molecules such as H₂, CO, and CH₄, as well as light char and tar type compounds. After decomposition, the pyrolysis-oil undergoes combustion, which practically provides all the thermal energy required to sustain the endothermic reactions. A series of endothermic reactions, including water gas, Boudouard, water gas shift, and steam methane-reforming reactions occur at this stage (Doherty *et al.* 2009). Useful combustible gases, such as H₂ and CO, are produced at

the gasification stage. At the end, the whole gasification process generates a syngas composed mainly of CO, CO₂, H₂, and CH₄. The production of CO, CO₂, CH₄, H₂, and steam in the whole process can be explained by the reactions given in Eqs. 1 to 8, which occur at various stages (Moghadam *et al.* 2014).



Clean ash-free syngas is an important intermediate product for many processes, such as those aimed at producing ammonia, hydrogen, methanol, and Fischer-Tropsch fuels. The syngas can also be used directly into fuel cells to generate heat and power (Tomasi *et al.* 2006). Pröll *et al.* (2007) investigated the use of syngas produced from gasification and successfully fed into a combined heat and electrical power (CHP) unit rated at 8 MW_{th}. The results demonstrated that CHP-concepts based on biomass steam gasification can reach high electric efficiencies and high fuel utilization rates (Pröll *et al.* 2007).

In this study, a model simulating syngas production *via* pyrolysis-oil gasification was developed, validated, and used to predict the effect of varying operating conditions on syngas properties. First, the modeling methodology is discussed, *i.e.*, the assumptions, the description, and the validation of the model. Thereafter, syngas potential applications in fuel cells and fuel productions are discussed. Lastly, the results are presented and discussed, highlighting the impacts of various operating conditions on syngas properties such as syngas composition, LHV, and H₂:CO molar ratio.

EXPERIMENTAL

The main purpose was to design a comprehensive process model for pyrolysis oil gasification, so that the model could be used as a predictive tool for the optimization of the gasifier performance. Operating parameters such as gasifying agent type (steam, oxygen, and air), temperature, and the oil moisture content were varied over wide ranges. The resulting syngas composition, LHV, and H₂:CO molar ratio were investigated. Although the gasifying pressure is also an important parameter that affects syngas composition, it was set to atmospheric pressure in this study for the purpose of avoiding costly equipment that would be required for higher pressures.

Assumptions

The whole model is based on the following assumptions:

- (1) Gasification is assumed to occur at steady state under isothermal and thermodynamic equilibrium conditions (Ramzan *et al.* 2011).
- (2) Pyrolysis-oil gasification occurs instantaneously, and the volatile products formed mainly consist of H₂, CO, CO₂, CH₄, H₂S, NH₃, and H₂O molecules.
- (3) All gases are ideal gases and are uniformly distributed in the gas phase.

Model Description

Based on the recommendation of the Aspen Plus user guide version 10.2 (Elan 1998), the Peng-Robinson equation of state with Boston-Mathias alpha function (PR-BM) was chosen to estimate the physical properties of the conventional components. The parameter alpha in PR-BM in the property package is a temperature-dependent variable (Elan 1998). The Peng-Robinson property method is suitable for non-polar and weakly polar mixtures, applicable to all temperature and pressure ranges. Therefore, this method was recommended for gas processing, refineries, and petrochemical applications. The enthalpy and density model selected for both pyrolysis-oils, are non-conventional components, HCOALGEN and DCOALIGT (Ramzan *et al.* 2011).

The process flow diagram (PFD) in Fig. 1 shows the Aspen Plus blocks used to simulate the gasification process. The model consists of four stages in the modelling: drying (RStoic), decomposition (RYield), combustion (RGibbs), and gasification (RGibbs) (Andrianopoulos *et al.* 2015). The description of Aspen Plus block is presented in Table 1. The pyrolysis-oil is specified as a non-conventional component and defined in the simulation model using the ultimate and proximate analysis of pyrolysis-oil. The NC (nonconventional) definition of pyrolysis-oil is shown in Appendix A. The data for pyrolysis-oil is given in Table 2 and was extracted from previous work presented in the literature (Rossum *et al.* 2007).

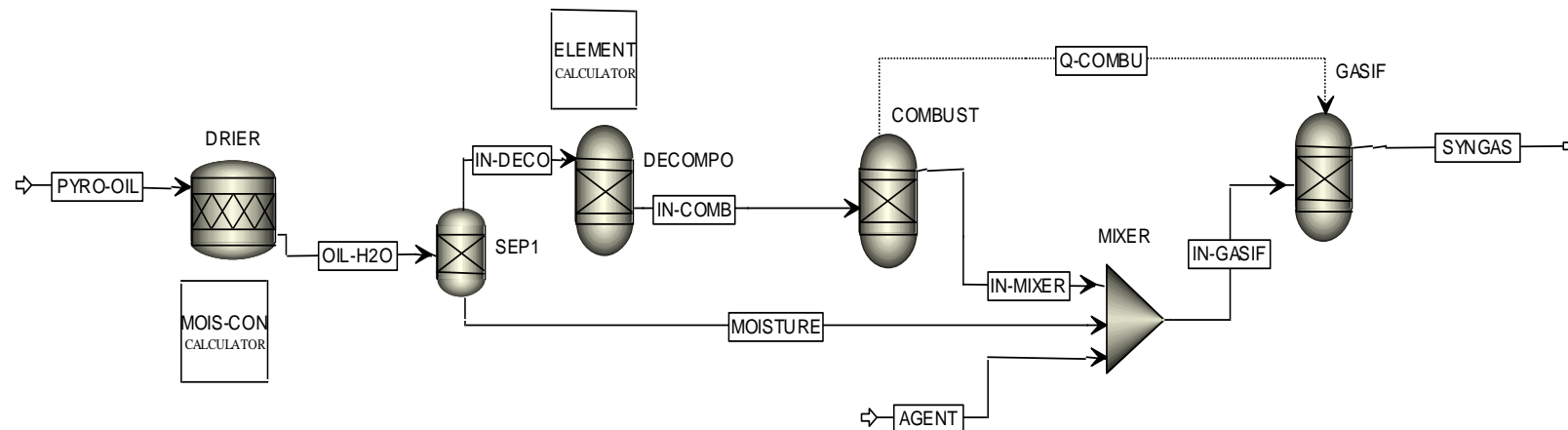
Table 1. Description of Blocks Used in the Gasification Model

Aspen Plus Block ID	Flowsheet Block ID	Description
*RStoic	DRIER	Reactor with known conversion rate - used to extract moisture from pyrolysis-oil. Operation at 150 °C.
Sep	SEP1	Used to separate moisture from the pyrolysis-oil.
RYield	DECOMPO	Yield reactor- used to decompose non-conventional pyrolysis-oil into its components by FORTRAN statement. Operation at 500 °C.
RGibbs	COMBUST	Gibbs free energy reactor- used to complete chemical equilibrium by minimizing Gibbs free energy. Operation at 800 °C.
Mixer	MIXER	Used to mix pyrolysis-oil and moisture
RGibbs	GASIF	Gibbs free energy reactor- used to calculate syngas composition by minimizing Gibbs free energy. Operation in the temperature range from 200 °C to 1200 °C.

*Drying Constant: 0.325 of pyrolysis-oil

Table 2. Pyrolysis-oil Composition Defined in Aspen Plus

Proximate analysis (wt%)	
Moisture content	32.5 - 43.7
Ultimate analysis (wt%)	
Carbon	30.4 - 37.7
Hydrogen	7.6 - 7.9
Nitrogen	< 0.01-0.27
Oxygen	54.4 - 61.7
Sulfur	< 0.01

**Fig. 1.** Aspen Plus simulation of pyrolysis-oil gasification process flow diagram

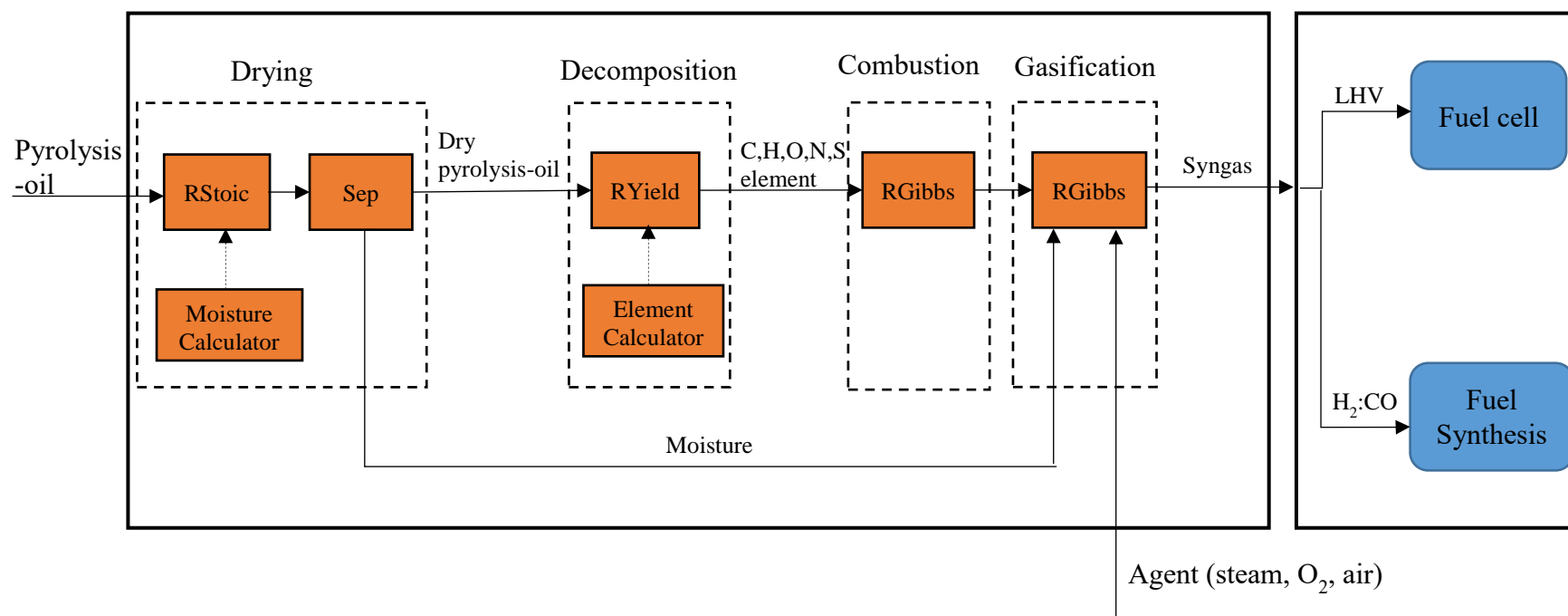


Fig. 2. Aspen Plus simulation calculation method and syngas potential application

A kinetic free equilibrium model was developed in Aspen Plus to simulate the gasification process through four stages. Aspen Plus simulation calculation method and syngas potential application are presented in Fig. 2. Firstly, the moisture was extracted from pyrolysis-oil, the pyrolysis-oil was fed into the RStoic block to model the drying process controlled by the FORTRAN statement in the calculator block that calculated the moisture content. In the next step, the dry oil was fed into a decomposition reactor where pyrolysis-oil decomposes into its elemental components (C, H, O, N, S, *etc.*), the distribution of which was specified using a FORTRAN statement in a calculator block according to the pyrolysis oil ultimate analysis. The RYield block is used to convert non-conventional pyrolysis-oil into conventional components by using FORTRAN statements in the calculator block. Then the combustion of pyrolysis oil is modeled by a Gibbs reactor. The RGibbs block handles the complete chemical equilibrium by minimizing the Gibbs free energy at an elevated temperature.

The decomposed pyrolysis-oil enters the RGibbs block where partial oxidation and combustion reactions occur. After combustion, the produced syngas was mixed with steam originating from pyrolysis-oil moisture in a MIXER block. The mixture was fed into the gasification unit. Lastly, gasification is also modeled using a Gibbs reactor. The RGibbs block handles the calculation of the syngas composition by minimizing Gibbs free energy (Begum *et al.* 2014). Afterward, the produced syngas will be applied in fuel cell or fuel production.

RESULTS AND DISCUSSION

The validated model is used alone with a sensitivity analysis to identify the effect of various operating conditions on syngas properties. The key parameters investigated in this analysis are the type of medium (gasifying agent), gasification temperature, and moisture content in pyrolysis-oil. The key syngas properties affected by the operating conditions and analyzed in this work are the syngas composition (given in mole fraction), the LHV and the H₂:CO molar ratio.

The LHV parameter represents the amount of heat released when a substance undergoes complete combustion with oxygen under standard conditions prior to condensation of water vapor produced. This parameter is meaningful when the generated syngas is used for energy applications, *e.g.*, as a feedstock for fuel cells to generate electricity and heat (combined heat and power unit). The higher LHV value, the higher electricity and heat produced from fuel cells. The LHV can be calculated as a function of the molar fraction of molecules in the gaseous mixture as follows (Moghadam *et al.* 2014),

$$LHV (MJ/Nm^3) = (CO \times 126.36 + H_2 \times 107.98 + CH_4 \times 358.18 + C_2H_2 \times 56)/1000 \quad (1)$$

If fuel synthesis applications are targeted, the main concern is the syngas composition (mole fraction of each element), with a particular focus on the H₂:CO molar ratio. For example, methanol synthesis and Fischer-Tropsch synthesis require a value of 2 for this ratio (Erena *et al.* 2005; Ma *et al.* 2015).

$$H_2:CO \text{ molar ratio} = n(H_2): n(CO) \approx 2 \quad (2)$$

Validation of Results

The flowsheet in Aspen Plus is presented in Appendix B. The simulation model was validated by using experimental data from a study achieved by Van Rossum *et al.* (2007) on the gasification of pyrolysis oil. A comparison between the experimental data and the simulation results is presented in Table 3. In the reference study, the pyrolysis oil was used to produce syngas through gasification in a fluidized bed with nickel-based catalysts at 800 °C. The modeled syngas concentration was in good agreement with the experimental results, except for the concentration of carbon monoxide (CO) and methane. The most noticeable discrepancy is the high amount of methane (5.1 mol%) obtained in the experiments, compared to the amount predicted by the model (0.3 mol%). This trend of excess methane with respect to thermodynamics is well known. The methane reforming reaction (Eq. 8) is limited by the reaction time. Therefore, it cannot reach the complete equilibrium state (Zhang *et al.* 2009). For the same reason, the actual amount of CO found in the gas phase is smaller than that simulated by the kinetic-free model (see Eq. 8). Nearly 90% carbon converted into syngas, the remaining carbon was converted into tar in Van Rossum research. In this research, tar was not defined in Aspen Plus, carbon was 100% converted into syngas. Table 4 also presented the energy consumption of pyrolysis oil gasification based on a flow rate of 100 kg/hr. As we can see that during the combustion stage, it releases 415.85 kW heat, which can be used for the gasification stage. The entire gasification process requires a total of 324.70 kW.

Table 3. Comparison between Experimental and Simulated Results

Syngas Composition (mole %)	Experiment (Van Rossum <i>et al.</i> 2007)	Model	Difference (Model - experiment)
H ₂	55.5	55.9	0.4
CO	19.3	24.0	4.7
CO ₂	19.0	19.8	0.8
CH ₄	5.4	0.3	-5.1
C ₂ H ₆	1.0	Trace	-
H ₂ S	-	Trace	-
NH ₃	-	Trace	-

Table 4. Energy Consumption for Each Stage

Case	Drying (150°C)	Decomposition (500°C)	Combustion (800°C)	Gasification (800°C)	Total
Energy Consumption (kW)	24.50	643.74	- 415.85	72.31	324.70

Effect of Operating Conditions

Effect of gasifying agents

The equivalence ratio is defined as the stoichiometric air/fuel ratio required for complete combustion. In this study, the equivalence ratio of agent (air, O₂, and steam) to pyrolysis-oil was set at 0.2. Runs were conducted with three gasifying agents, *i.e.*, oxygen, steam, and air. The specific syngas yield with gasifying agents is presented in Appendix C. Figure 3 presents the syngas composition for each gasifying agent used in the process. Figure 4 presents the LHV and H₂:CO molar ratio for each gasifying agent. Syngas produced with steam had the highest content in hydrogen (53.3 mol%) and CO (33.0

mol%). As a result, the syngas LHV is also highest (9.89 MJ/Nm³) in this configuration. Gasifying with oxygen leads to a smaller LHV because oxygen reacts with H₂ and CO within the mixture. However, the H₂:CO molar ratio was higher when gasifying with oxygen (1.85) compared to gasifying with steam (1.61). The higher H₂:CO molar ratio is favorable for fuel synthesis. Finally, gasifying with air leads the lowest LHV (7.94 MJ/Nm³), because oxygen is diluted to 21% in this agent, the balance being mostly inert nitrogen. This trend of LHV variation as a function of gasifying agent is in good agreement with experimental results from Gil *et al.* (1999), where three types of gasifying agents were used in biomass gasification and the syngas distribution were tested. The H₂-content in the syngas was highest when steam was used as gasifying agent. Gasifying with air led to the lowest syngas LHV.

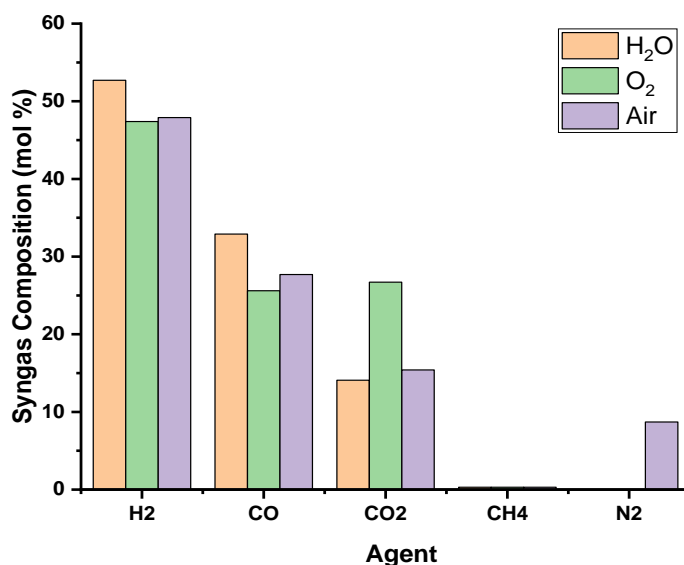


Fig. 3. Effect of gasifying agent on syngas composition (at 800 °C)

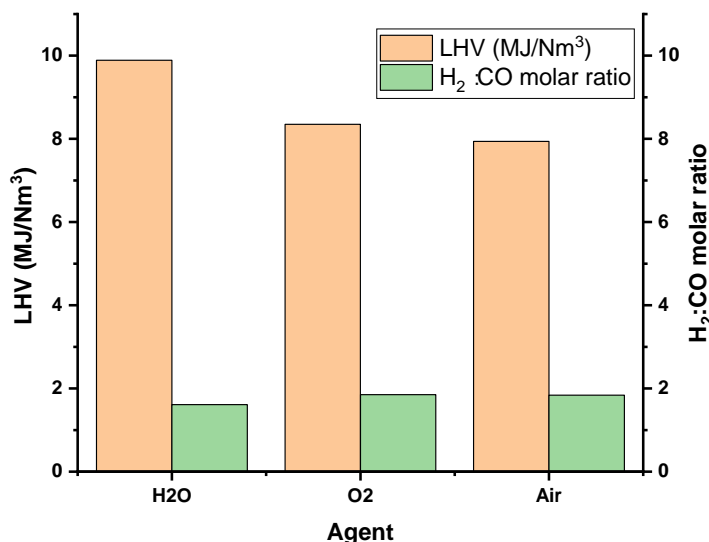


Fig. 4. Effect of gasifying agent on syngas LHV and H₂:CO molar ratio (at 800 °C)

Effect of gasifying temperature

The gasification temperature is an influential parameter in syngas production. Figures 5 and 6 show the effect of temperature on syngas composition, LHV, and H₂:CO ratio. The gasifier temperature ranged from 200 °C to 1200 °C. At low temperatures, the syngas was composed mainly of methane and CO. The concentration of methane decreased with increasing gasifier temperature from 200 °C to 600 °C. This decrease was due to the steam methane reforming reaction (Eq. 8), which converts methane into hydrogen and CO. The carbon and hydrogen in pyrolysis-oil were not completely converted into syngas at low temperature. However, when the temperature was increased from 200 °C to 800 °C, the content of CO and hydrogen greatly increased. This trend is consistent with Boudouard (Eq. 4) and water gas (Eq. 6) reactions, *i.e.*, the carbon in pyrolysis-oil reacts with water and CO₂ to generate hydrogen and CO. The carbon dioxide content thus decreased with increasing temperature. High operating temperatures favor the production of hydrogen and CO. The H₂:CO molar ratio reached a maximum of 2.41 at 600 °C, and then gradually decreased with increasing temperature within this range. At high temperatures (above 800 °C), the concentrations of hydrogen and CO₂ decreased slightly, while the concentration of CO slightly increased. This trend was attributed to the water gas shift reaction (Eq. 7) that is thermodynamically unfavorable. Due to its exothermic nature, this reaction is thermodynamically favored at lower temperature. The syngas LHV continuously increased (first rapidly, then slightly) as the gasifier temperature was increased, leading to higher production of CO and to a syngas LHV of 9.51 MJ/Nm³ at 1200 °C. The trend of H₂ and CO concentration, syngas LHV value and H₂:CO molar ratio was in good agreement with Dai study (Dai *et al.* 2019). In his research, the H₂ concentration increases with increasing temperature and then decreases slightly. Syngas LHV value increases as the gasifying temperature increase. Syngas producing from high temperature is beneficial to fuel cells applications and harmful to fuel synthesis.

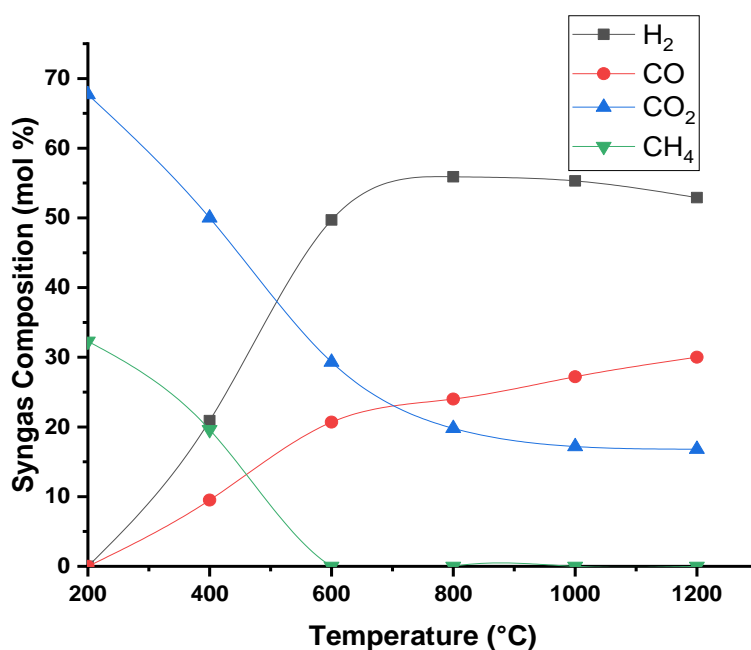


Fig. 5. Effect of gasifier temperature on syngas composition

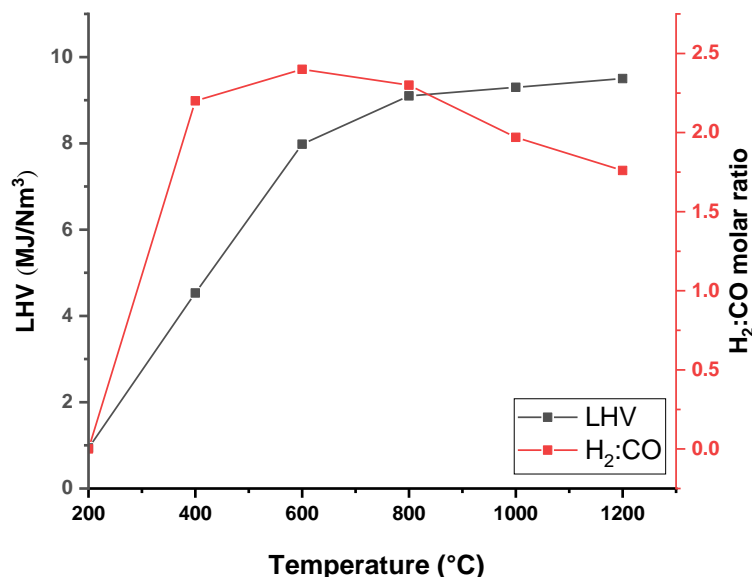


Fig. 6. Effect of gasifier temperature on syngas LHV and H₂:CO molar ratio

Effect of moisture content in pyrolysis oil

Figures 7 and 8 present the effects of pyrolysis-oil moisture content (from 10 wt% to 50 wt%), H₂:CO molar ratio, and LHV on syngas composition.

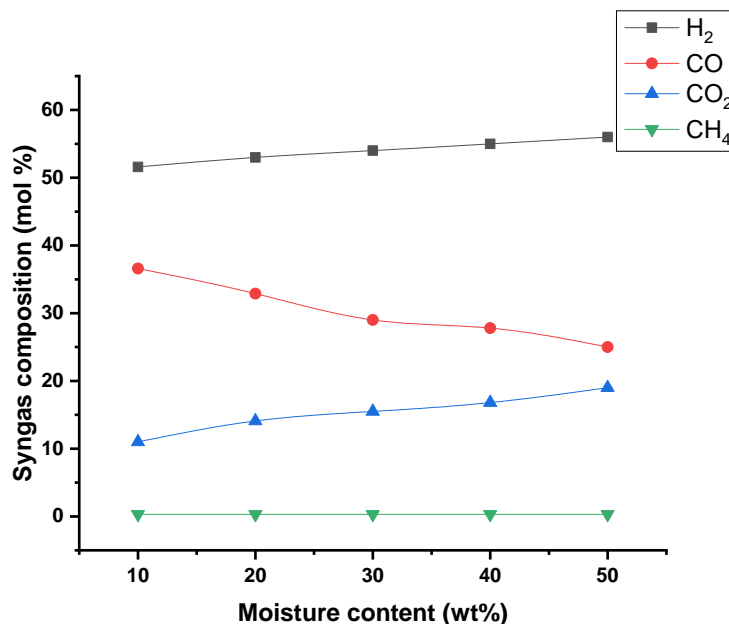


Fig. 7. Effect of pyrolysis oil moisture content on syngas composition (at 800 °C)

According to the water gas shift (Eq. 7) and water gas reactions (Eq. 6), an increasing moisture content led to an increase in the mole fractions of H₂ and CO, and a decrease in the amount of carbon monoxide. As a result, the H₂:CO molar ratio gradually increased from a minimum of 1.5 to a maximum of 2.24 at 50 wt% moisture content.

However, the LHV decreased from 10.1 to 9.2 MJ/Nm³ over the same range, due to the decrease in CO content. Therefore, if energy applications are targeted (heat and power generation), then the moisture content in pyrolysis-oil should be kept low. If fuel synthesis (*e.g.*, methanol or Fischer-Tropsch fuels) is targeted, then the moisture content can be optimized at 40% to adjust the syngas composition, especially the H₂:CO molar ratio.

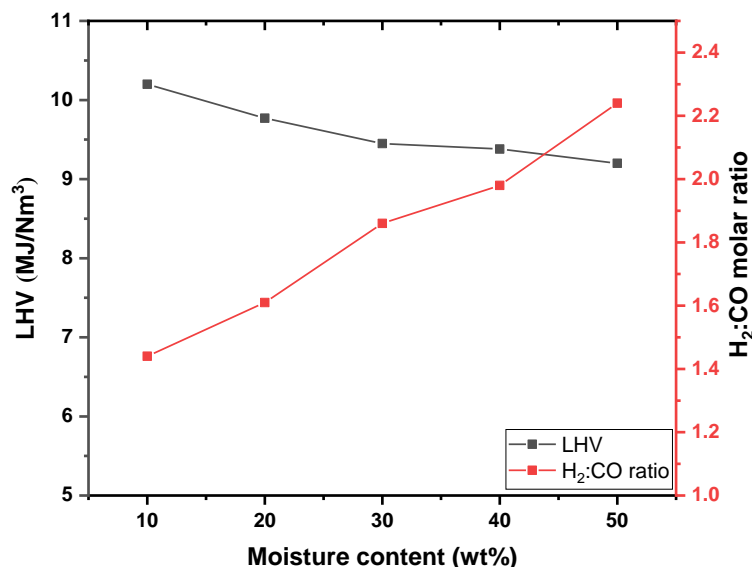


Fig. 8. Effect of pyrolysis-oil moisture content on syngas LHV and H₂:CO molar ratio (at 800 °C)

CONCLUSIONS

1. The objective of this study was to develop a model to simulate and predict the steady state performance of the pyrolysis-oil gasification process. The results obtained from simulation are in good agreement with experimental data from literature. Therefore, the model can predict the gasification performance over a wide range of operating conditions. The influence of various gasification agents was investigated by using a fixed equivalence ratio at 800 °C. At these conditions, the syngas LHV was maximized at 9.89 MJ/Nm³ by using steam as agent. High temperature favors to the production of CO, which results in high syngas LHV (9.51 MJ/Nm³). High moisture content in pyrolysis-oil leads to a syngas that is rich in hydrogen, but poor in CO content. As a result, the syngas LHV decreased with increasing moisture content in pyrolysis-oil, but the H₂:CO molar ratio increased to 2.24 wt% at 50 wt% moisture content in pyrolysis oil.
2. If the syngas is applied to fuel cells to generate heat and electricity, then the O₂ and air cannot be used as agent, which can reduce the LHV value of the syngas. Moisture content in pyrolysis-oil should be minimized. The syngas should also be produced at a high temperature for this application since it then has a higher enthalpy value that can potentially generate more electricity and heat.
3. If the syngas is used for methanol synthesis or Fischer-Tropsch fuel production, then a small amount of O₂ can be used to adjust the H₂:CO molar ratio. The syngas should be

produced at 1000°C where H₂:CO molar ratio equal to 2. An appropriate amount of moisture content in pyrolysis oil should be selected at 40%.

4. Syngas produced from pyrolysis oil contains less nitrogen oxides and sulfur dioxide, making the syngas more suitable to fuel cells or fuel production processes. Therefore, pyrolysis oil provides a sustainable energy pathway from forest resources to a biofuel that can be used in the fuel cells, which can be deployed in the remote and off-grid communities to provide heat and electricity. Besides that, the use of pyrolysis oil generated from forest resources would help reducing our dependency on fossil fuels and cutting down greenhouse -gases emissions.

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Appendix A

Pyrolysis-oil NC definition

Attribute ID:			
PROXANAL		SULFANAL	
MOISTURE	32.5	PYRITIC	0.001
FC		SULFATE	
VM		ORGANIC	
ASH			

Appendix B

Flowsheet in Aspen Plus

Component Mass flow (kg/hr)	Pyro-oil	Oil-H ₂ O	IN-DECO	MOISTURE	IN-COMB	IN-MIXER	IN-GASIF	SYNGAS
Pyrolysis oil	100							
Oil		67.5	67.5					
H ₂ O		32.5		32.5			32.5	
*H ₂					4.15			
*O ₂					32.82			
*C					30.40			
*N ₂					0.27			
*S					0.001			
H ₂ O						trace	trace	4.27
H ₂						4.09	4.09	6.42
CO						57.01	57.01	38.60
CO ₂						trace	trace	50.04
CH ₄						0.29	0.29	0.28
C						5.97	5.97	
H ₂ S						0.001	0.001	trace
H ₃ N						0.38	0.38	0.33
C ₂ H ₆						trace	trace	trace

*Elemental distribution

Appendix C

Effect of gasifying agents (800°C)

Component Mass flow (kg/hr)	Pyro-oil	Oil- H ₂ O	IN-DECO	MOISTURE	IN-COMB	IN- MIXER	AGENT			SYNGAS		
							Steam	Air	O ₂	Steam	Air	O ₂
Pyrolysis oil (20% moisture content)	84.4											
Oil		67.5	67.5									
H ₂ O		16.9		16.9			13.5					
H ₂					4.15							
O ₂					32.82			2.8	13.5			
C					30.40							
N ₂					0.27			10.7				
S					0.001							
H ₂ O						trace				9.46	trace	2.08
H ₂						4.09				5.64	5.21	4.50
CO						57.01				49.46	43.07	34.3
CO ₂						trace				32.96	38.88	56.87
CH ₄						0.29				0.253	0.009	trace
C (Pure Solid)						5.957						
H ₂ S						0.001				trace	trace	trace
H ₃ N						0.38				0.32	0.32	0.32
C ₂ H ₆						trace				trace	trace	trace
N ₂												10.7