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Simulation of Integrated Pressurized Steam Gasification of Biomass for Hydrogen Production using iCON

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Abstract: Energy in the form of biomass has been used to produce heat, electricity, steam and petrochemicals due to the zero net carbon emission. With regards to the environmental concerns, hydrogen offers a competitive edge over the fossil fuel as an alternative clean energy. Currently, production of hydrogen from biomass using a pressurized system is not being extensively analyzed and developed. Thus, process and flowsheet development of pressurized gasification process of biomass coupled with carbon dioxide adsorption for hydrogen production were investigated using a PETRONAS iCON simulation model. The effect of parameters such as pressure, temperature and steam/biomass ratio on the hydrogen yield was investigated. Hydrogen yield was predicted to be increasing with pressure, temperature and steam/biomass ratio in this high pressure gasification system.

Key words: Biomass, pressurized gasification, hydrogen, iCON

INTRODUCTION

With the current energy crisis and moreover, the fluctuating price of fossil fuel, biomass is one of the potential solutions to the problem. Production of energy from biomass is sustainable and environment-friendly featured by its low SO_2 emissions, no carbon footprint due to photosynthesis (Holladay *et al*., 2009) and short rotation forestry. Furthermore, biomass is reported to contribute in green industries with associated growth in rural economies (Levin and Chahine, 2010). Its utilization to produce energy can contribute significantly towards the objective of the Kyoto Agreement in reducing the green house gases emissions and problems related to climate change (Ni *et al*., 2006). Other than these factors, biomass is abundantly available at low costs and could also be supplied easily compared to other natural resources in Malaysia, a major palm oil producer.

Biomass can be converted into hydrogen and other gases such as methane, carbon monoxide and carbon dioxide, via bio-chemical and thermo-chemical gasification processes (Kumar *et al*., 2009). Bio-chemical gasification refers to the gasification by microorganism at normal temperature and pressure while thermo-chemical gasification requires the use of air, oxygen or steam at temperature more than 800°C (McKendry, 2002). Thermo-chemical gasification produces a product gas, containing hydrogen or value-added by-products such as methane. Biomass could be readily gasified to produce high purity hydrogen gas. Hydrogen produced from biomass is a type of clean energy with zero net carbon emissions and could be readily used in most of the present energy conversion systems for natural gas derived hydrogen as well as advanced power generation devices such as fuel cells (Kalinci *et al*., 2009). Gasification technology has advanced significantly from time to time in order to meet the demand of lowest cost of production and higher production rate. One of the improvements available is to incorporate carbon dioxide removal step in the gasification process or to conduct the gasification at high pressure (Florin and Harris, 2008).

Fermoso *et al*. (2009) performed an experimental work on the gasification of a mixture of coal, biomass and petroleum coke with the feed particle size of 75-150 μm at 1 MPa. They reported that hydrogen and methane compositions in the product gas were almost constant when the reaction temperature was increased. Hydrogen and carbon monoxide productions were reported to be decreasing with increasing pressure while methane and carbon dioxide depicted increasing trends. Mahishi and Goswami (2007) conducted a thermodynamic analysis of hydrogen production from biomass using equilibrium modeling. However, they reported that pressure did not have significant effect on the increment of hydrogen

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amount in the product gas near to atmospheric pressure. Meanwhile, Hanaoka *et al*. (2004) conducted a gasification experiment at high pressure using woody biomass and steam together, incorporated with the carbon dioxide removal unit. They reported that at pressure of 0.6-0.7 MPa, hydrogen yield increased with temperature. The highest hydrogen yield was predicted at 0.6 MPa.

In addition, Florin and Harris (2008) investigated on a system of gasification combined with carbon dioxide removal. Based on their results through modelling, they reported that hydrogen yield was increasing with temperature. Hydrogen yield also displayed the same trend of increment corresponding to the steam/biomass ratio. Meanwhile, the overall hydrogen production was observed to increase with pressure. Since the hydrogen production from biomass via pressurized gasification that is coupled with carbon dioxide adsorption has not been widely investigated and there are limited models to represent the case, this paper hence aims to develop a simulation model for such a system and predict its performance via simulation approach. In this study, a simulation model is developed in PETRONAS iCON process simulator and is used to investigate the technical feasibility of the biomass pressurized gasification system based on the effect of parameters such as pressure, temperature and steam/biomass ratio on the product gas composition and hydrogen yield.

MATERIALS AND METHODS

Reaction schemes: The reactions assumed to occur in the integrated gasification unit are listed in Table 1, along with the corresponding stoichiometric equations and heat of reactions.

Gasifying agent: In this process model, steam is used as the gasifying agent in order to obtain higher hydrogen yield and lower solid residues (Jangsawang *et al*., 2006). Gonzalez *et al*. (2008) observed that the solid amount produced from steam gasification was significantly lower with higher impact of temperature variations i.e., 28 to 6%, compared to 23 to 18% solid from air gasification for the temperature range between 700 and 900°C. In the same study (Gonzalez *et al*., 2008), the hydrogen yield for steam gasification was observed to increase considerably from 8 to 33% compared to decrement observed for air gasification from 9 to 5% for temperature range of 700 to 900°C.

CO_2 capture technique: In order to increase the hydrogen purity in the product gas, the CO_2 capture technique has been employed within the system, with CaO as sorbent. CaO played dual role, as absorbent and catalyst by moving gasification reactions in forward direction (Florin and Harris, 2008). Furthermore, overall energy consumption is reduced due to the exothermic behavior of carbonation reaction.

Table 1: Reaction scheme in the integrated steam gasification unit (Inayat *et al*., 2010b)

No.	Name	Reaction	Standard heat of reaction (kJ moL^{-1})
R1	Char gasification	$C + H_2O \rightarrow CO + H_2$	131.5
R2	Methanation	$C + 2H_2 \rightarrow CH_4$	-74.8
R3	Methane reforming	$CH_4 + H_2O \rightarrow CO + 3H_2$	206.0
R4	Water gas shift	$CO + H_2O \leftrightarrow CO_2 + H_2$	-41.0
R5	Carbonation	$CO_2 + CaO \rightarrow CaCO_3$	-178.0
R6	Boudouard	$C + CO_2 \rightarrow 2CO$	172.0

Reaction kinetics: The compilation and the basis of selection of relevant kinetics adapted from relevant literatures for the pressurized integrated steam gasification are given in Table 2.

For reactions R2 (methanation), R3 (methane reforming) and R6 (Boudouard), the kinetics is adapted from Lu *et al*. (2008) who investigated biomass gasification. As the same kinetics representation was applied by Macak and Malecha (1978) for a gasification system operating at a high pressure of 2.648 MPa, even though for coal, the same kinetics is used in this work. Hence, for reactions R1 (carbon gasification) and R4 (water gas shift), the kinetics model proposed by Lu *et al*. (2008) is also adapted due to the same reasons. Carbonation kinetics is adapted from the study by Lee *et al*. (2004) in which the operating pressure reported are 3, 7 and 15 bar.

Process assumptions: Assumptions made in the simulation are:

- Biomass (wood) is represented as pure char (Gobel *et al*., 2007)
- The reactions occur sequentially and are in isothermal condition (Shen *et al*., 2008)
- The system is under steady state conditions (Inayat *et al*., 2010a; Zhang *et al*., 2009)
- Carbonation is assumed to be a forward reaction within the temperature range used (Yunus *et al*., 2010)
- Ash is an inert hence does not participate in the reactions (Nikoo and Mahinpey, 2008)
- Tar formation is negligible (Paviet *et al*., 2009)

Process development: The biomass pressurized gasification process is assumed to consist of reactions R1 to R6 occurring in sequence as shown in Table 1. The process flow diagram of the gasification system is shown in Fig. 1.

Table 2: Kinetics of reactions in the integrated steam gasification unit

Reaction	Kinetics constant (m/h)	Reference
Char gasification	$1.05\times10^{7}\ \exp\ (\frac{-232000}{RT})$	Lu *et al.* (2008), Macak and Malecha (1978)
Methanation	$21\times10^{3}\ \exp\ (\frac{-230274}{RT})$	Lu *et al.* (2008), Macak and Malecha (1978), Raman *et al.* (1981)
Methane reforming	$2.0\times10^{7}\ \exp\ (\frac{-360065}{RT})$	Macak and Malecha (1978), Raman *et al.* (1981)
Water gas shift*	$7.0\times10^{3}\ \exp\ (\frac{-30000}{RT})$	Lu *et al.* (2008)
Carbonation	$96.34\ \exp\ (\frac{-101189}{RT})$	Lee *et al.* (2004)
Boudouard	$1.0\times10^{7}\ \exp\ (\frac{-12560}{RT})$	Lu *et al.* (2008), Macak and Malecha (1978), Raman *et al.* (1981)

*m^3/kmol: h

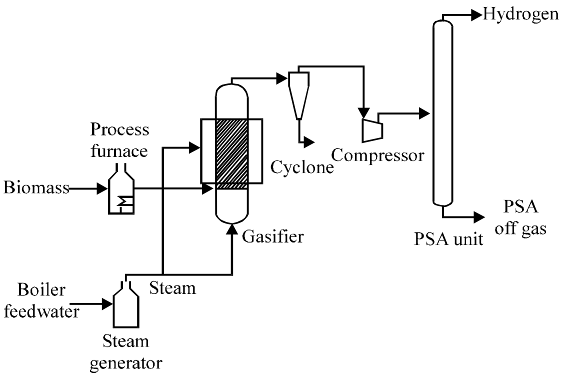

Fig. 1: Process flow diagram

RESULTS AND DISCUSSION

Process simulation in iCON: Biomass is dried and pelletized before it is being fed into the gasifier. Since this is a high pressure unit, compression of steam needs to be done before being fed into the gasification unit. The biomass gasification is assumed to occur in the gasification unit along with the carbon dioxide capture. Reactions assumed to occur in the gasification unit include char gasification, methanation, methane reforming water gas shift, boudouard and carbonation. The product gas is next being treated in the Pressure Swing Adsorption (PSA) unit to get pure hydrogen gas.

iCON is a commercial process simulator developed via a collaboration effort between PETRONAS and Virtual Materials Group (VMG) Inc. The engine is based on Sim42, an open source process simulator and runs on VMGThermo as the plug-in thermodynamics property package database standard. The Gasification property package is used in the simulation to incorporate gasification properties along with solid support. Figure 2 shows the iCON simulation snapshot of the gasification process incorporating the carbon dioxide removal step while Table 3 shows the streams data and the operating conditions for the gasification process.

Effect of temperature: For the high pressure gasification system shown in Fig. 3, hydrogen amount in product gas increases with increasing temperature. This observation matches the findings published by Hanaoka *et al.* (2004) and Fermoso *et al.* (2009). Figure 3 also plots the composition of each component in the product gas with respect to change in temperature while Fig. 4 shows the effect of temperature on hydrogen yield.

Based on Fig. 3, it can be seen that carbon monoxide amount decreases with the temperature rise from 1200°C to 1500°C. Changes in the amount of methane and carbon dioxide produced are negligible with the temperature increment. The reason behind these observations is high temperature promotes the endothermic reactions of char gasification, methane reforming and boudouard.

With these three reactions being enhanced, more hydrogen is produced. Meanwhile, high temperature also induces the reverse of water gas shift reactions leading to lesser carbon monoxide amount produced in the system, however, the carbon dioxide removal promotes the water gas shift reaction forward (Fig. 4).

Effect of pressure: It is observed that hydrogen amount in the high pressure system is in the increasing trend with pressure. This profile matches the findings reported by Florin and Harris (2008) and Mahishi and Goswami (2007). Figure 5 shows hydrogen amount increases with pressure while carbon monoxide amount decreases. The simulation also predicts negligible amounts of carbon dioxide and methane.

Similarly, Fig. 6 shows that hydrogen yield increases with pressure. When pressure is increased, biomass is gasified faster with the same heat being supplied to the system due to the increased char surface area (Roberts and Harris, 2000). Thus, more hydrogen is produced.

Effect of steam/biomass ratio: Figure 7 shows that hydrogen amount produced using the high pressure system is increasing with increasing steam/biomass ratio. This trend is similar to that observed by Florin and Harris (2008).

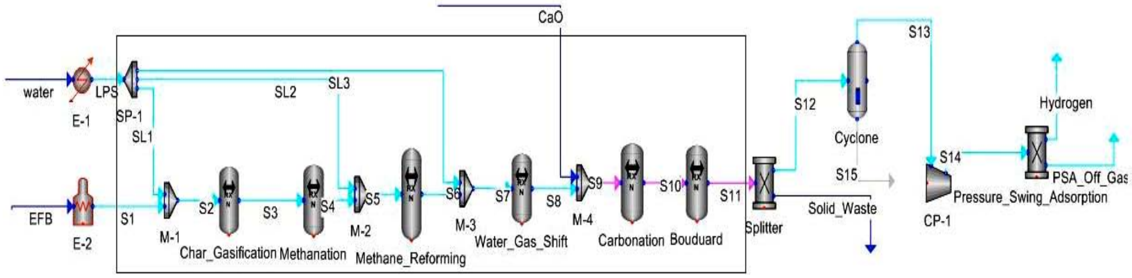

Fig. 2: Snapshot of the iCON simulation model for the biomass pressured integrated gasification system

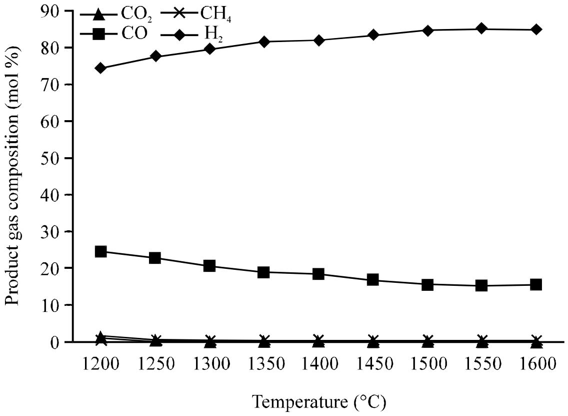

Fig. 3: Effect of temperature on product gas composition. Steam/biomass ratio: 2.45; Pressure: 800 kPa

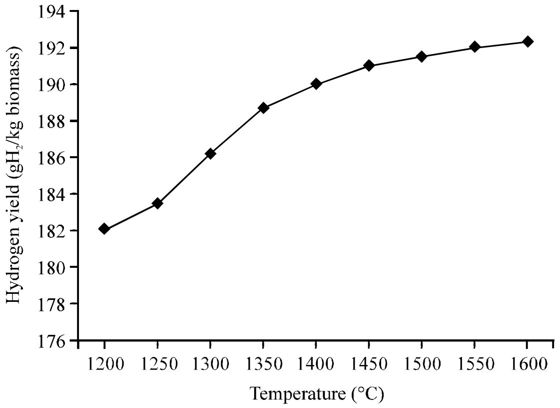

Fig. 4: Effect of temperature on hydrogen yield. Steam/biomass ratio: 2.45; Pressure: 800 kPa

As shown in Fig. 8, the hydrogen yield is predicted to increase with the increase in steam/biomass ratio. When more steam is being fed into the system, char gasification, methane reforming and water gas shift reactions are promoted. With these reactions being pushed forward, it leads to an increased production of hydrogen. The carbon dioxide removal step further promotes the water gas shift reaction forward, based on Le Chatelier's principle (Lu *et al*., 2010).

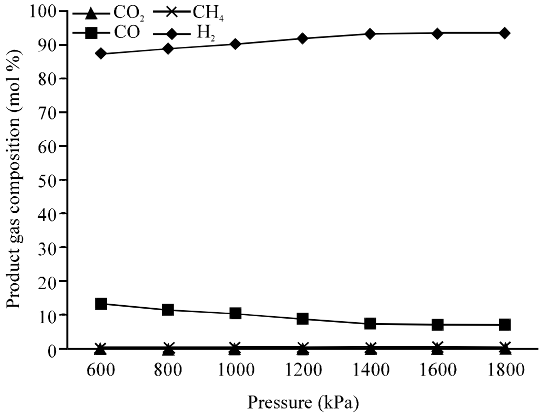

Fig. 5: Effect of pressure on product gas composition. Steam/biomass ratio: 2.45; Temperature: 850°C

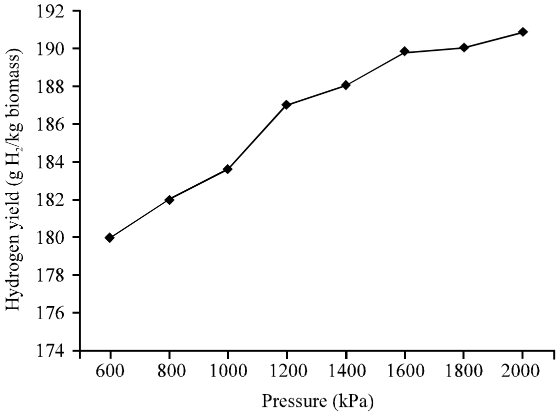

Fig. 6: Effect of pressure on hydrogen yield. Steam/biomass ratio: 2.45; Temperature: 850°C

Table 3: Operating parameters and mass fraction of components in the biomass pressured integrated gasification process

Name	CaO	EFB	H_2	LPS	PSA	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10	S11	S12	S13	S14	S15	SL1	SL2	SL3	Solid Waste	Water
T[°C]	850	300	850	850	850	850	850	850	850	850	850	850	850	850	850	850	850	850	850	850	850	850	850	850	25
P[kPa]	600	600	700	600	700	600	600	600	600	600	600	600	600	600	600	600	600	600	700	600	600	600	600	600	600
Mass Flow [kg/h]	4000	4000	1664	2400	1603	4000	4050	4051	4051	4969	4969	6401	6401	10401	10401	10401	3268	3268	3268	0	50	918	1432	7133	2400
Mass fraction																									
H_2O	0.00	0.00	0.00	1.00	0.49	0.00	0.01	4E-04	0.01	0.18	0.19	0.37	0.12	0.07	0.07	0.07	0.24	0.24	0.24	0.08	1.00	1.00	1.00	0.00	1.00
H_2	0.00	0.00	0.16	0.00	0.00	0.00	0.00	0.02	0.02	0.02	0.02	0.01	0.04	0.027	0.02	0.02	0.08	0.08	0.08	0.01	0.00	0.00	0.00	0.00	0.00
CO	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.62	0.62	0.51	0.49	0.38	3E-04	2E-04	2E-04	5E-04	0.01	0.01	0.01	0.13	0.00	0.00	0.00	0.00	0.00
CO_2	0.00	0.00	0.00	0.00	0.47	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.60	0.37	0.07	0.07	0.23	0.23	0.23	0.21	0.00	0.00	0.00	0.00	0.00
CH_4	0.00	0.00	0.00	0.00	0.02	0.00	0.00	0.00	8E-04	6E-04	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.07	0.00	0.00	0.00	0.00	0.00
CaO	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.38	6E-04	6E-04	0.00	0.00	0.00	0.00	0.00	0.00	0.00	9E-04	0.00
$CaCO_3$	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.68	0.68	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.99	0.00
Biomass	0.00	1.00	0.83	0.00	0.00	1.00	0.98	0.34	0.34	0.27	0.27	0.21	0.21	0.13	0.13	0.13	0.42	0.42	0.42	0.47	0.00	0.00	0.00	0.00	0.00

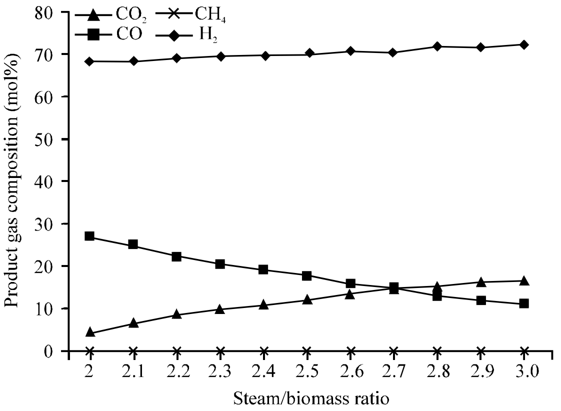

Fig. 7: Effect of steam/biomass ratio on product gas composition. Pressure: 800 kPa; Temperature: 850°C

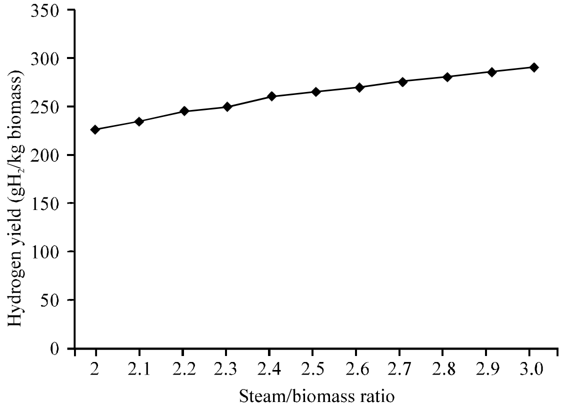

Fig. 8: Effect of steam/biomass ratio on hydrogen yield. Pressure: 800 kPa; Temperature: 850°C

Comparison with literatures: A results comparison from the current study for product gas composition has been done with published data on pressurized air-steam gasification without CO_2 capture step (Mahishi and Goswami, 2007) as shown in Table 4.

Table 4: Results comparison with literature

Basis	Mahishi and Goswami (2007)	Present study
Biomass	Wood	Wood
Approach	Equilibrium	Kinetics
Gasification agent	Steam	Steam
Pressure (kPa)	1010	1000
Temperature (°C)	827	850
Steam/biomass	1	2.45
Product gas composition (mol %)		
H_2	52.1	89.6
CO	30.3	9.2
CO_2	13.7	0.9
CH_4	3.9	0.3

The results show that current study predicts higher hydrogen production compared to the results reported by Mahishi and Goswami (2007). The comparison also proves that the hydrogen concentration is higher in steam gasification system with CO_2 capture step rather than other conventional gasification system. This is due to the use of CaO in the system which acts as sorbent and catalyst (Lu *et al.*, 2010).

CONCLUSION

The model of enhanced biomass gasification in high pressure steam-assisted gasifier is successfully developed and simulated in PETRONAS iCON. The results obtained show good agreement and follow empirical trends in referred literatures. The model predicts that for the biomass pressurized gasification process incorporating the carbon dioxide removal step, the higher the temperature, pressure and steam/biomass ratio, the higher hydrogen is being yielded. This study produces a good fundamental model to further develop the pressurized integrated gasification process for commercial purposes. Moreover, the flowsheet of the hydrogen production from biomass gasification can be further improved and optimized for better production yield with competitive cost. Experiments can also be performed in order to generate more applicable reaction kinetics that can further assist in the simulation work. Exact chemical formula for biomass should be used to produce more accurate predictions.

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