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Simulation of *Jatropha curcas* shell in gasifier for synthesis gas and hydrogen production

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ABSTRACT

This paper examines a simulation of *Jatropha curcas* shell within an entrained flow gasifier to predict the composition of gaseous product. Since there is no available data of Jatropha shell experiment, we validated the model using other biomass: rice husk and sawdust. The validation results showed that the model agreed with the experimental data of rice husk and sawdust. Furthermore, the same model is applied for *Jatropha curcas* properties data. From this simulation, we obtained that carbon monoxide (CO) and hydrogen (H_2) increased when reactor temperature was raised. Meanwhile, carbon dioxide (CO_2) and methane (CH_4) decreased. Since the simulation is not validated directly with Jatropha shell experimental data, error may come because of this situation. Therefore, we applied the Mean Error Approach (MEA) and produced a range of gas products through Jatropha shell in a simulation. The MEA data shows that methane (CH_4) has the highest mean errors with both sawdust and rice husk, at values of 0.8776 and 0.6115, respectively. Carbon monoxide (CO) on the other hand, has the lowest error. When we then apply this MEA to Jatropha shell simulation result, it shows that the range of carbon dioxide (CO_2) produced by Jatropha shell gasification has a composition ranging from 40.54 to 52.32% at a temperature of 1000 °C. The composition ranges of hydrogen (H_2), carbon dioxide (CO_2), and methane (CH_4) gases are 27.07–35.91%, 5.43–28.29%, and 0.49–9.96%, respectively.

1. Introduction

As climate change becomes an increasingly relevant issue, renewable energy sources such as biomass are looked to as options that reduce carbon emissions [1–4]. One biomass option is *Jatropha curcas Lynn*, which has been widely cultivated for industrial energy production in several countries including Indonesia [5–8], Thailand [9,10], India [11–13], Nicaragua [14], China [15] and Vietnam [16]. *Jatropha curcas Lynn* is a particularly good choice of biofuel because of its ability to produce adequate harvests from marginal soil [17,18]. Therefore, *Jatropha curcas Lynn* does not compete with food crops such as rice, potatoes and wheat, avoiding concerns about food security. Another advantage of *Jatropha curcas Lynn* is its drought resistance [19].

A number of Asian countries are projected to produce large amounts of *Jatropha curcas* Lynn seed over the coming years as shown in Fig. 1. These projections are based on the area of cultivation announced at the International Jatropha Organization and on projected seed production [20]. The foremost expected producer is China, which is predicted to harvest 19,050,000 tons of the oil in 2017. In that same year, India will produce another 16,750,000 tons, taking into account the country's official cultivation plan (the National Program on Jatropha). Indonesia's government has also announced a production plan, the Blueprint of Biofuel, and it is predicted to produce 6,570,000 tons. Myanmar, according to its National Jatropha Programme, is set to produce 4,250,000 tons of jatropha oil. Several other countries will

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produce much smaller amounts. Thailand, for instance, is expected to produce about 300,000 tons, the Philippines to produce 18,000 tons, and Malaysia 8000 tons. Cambodia, Nepal, and Vietnam are expected to produce roughly 2000 tons each. Other countries, such as Japan, are not predicted to produce any at all.

The energy production process most often involves conversion of *Jatropha curcas Lynn* seed into bio-oil which is widely used in a biodiesel blend. This oil is produced through several processes as shown in Fig. 2. It begins with seed collection. The seeds are then sent to a cracker machine. From this machine, *Jatropha curcas Lynn* kernels emerge, along with a byproduct of shells. The kernels are sent on to an extraction process, which produces Crude Jatropha Oil and a byproduct called oil cake seed. Because of the abundance of *Jatropha curcas* shell produced during this oil conversion processes, it is also can be considered as an energy source. This shell can be burned directly to produce heat. Several researchers have investigated a conversion of Jatropha shell into activated carbon and bio-briquette [21–23]. It can also be converted into a synthetic gaseous product through a gasification process, which produces more versatile products [24]. The gasification of this shell seems more advantageous than other methods of energy conversion. However there has been a lack of both simulation and experimental analyses. Therefore this paper will examine *Jatropha curcas* shell processed in the gasification reactor to understand the content of gaseous products. Similar research with a similar approach has been conducted on Jatropha oil seed cake from same author [25]. However, here we use Jatropha shell waste that is also abundant after oil extraction processes.

2. Gasification processes

Gasification is one of the most effective methods of energy conversion from biomass, and is one of the chemical conversion processes with the highest thermal efficiency [26,27]. This proven, robust technology can be operated either as a simple system using a fixed-bed gasifier or as a more sophisticated system involving fluidized-bed technology [24]. During gasification, a synthetic gas is produced through chemical mechanisms in several processes, in which the biofuel passes through a feeding system, a reactor, a cleaning system, and a cooling system. The reactor controls oxygen to avoid combustion while gasifying biomass at high temperatures. As mentioned, biomass gasifiers are classified into two main types, the simpler fixed-bed and more sophisticated fluidized bed. Fixed-bed gasifiers are further classified based on the relative directions of biomass and air flow into updraft, downdraft, and cross-draft categories. The sub-categories for fluidized bed gasifiers are based on the mode of fluidization, which is either bubbling or circulating [28]. The four processes that occur during gasification are drying, pyrolysis, oxidation, and reduction [29].

The reactions in the gasification process are presented in Table 1. The gasification process avoids combustion reactions, but amounts of carbon fixed from feedstock may react with oxygen and produce carbon dioxide (CO_2) and perform complete or partial combustion (see Table 1, reactions 1 and 2). This combustion reaction is exothermic and requires heat from the surrounding heater. Other forms of reaction in oxidation include steam production and CO oxidation (see Table 1 reactions 3 and 4). In steam production, Hydrogen (H_2) reacts with oxygen, while in CO oxidation Carbon monoxide (CO) reacts with oxygen. Both of these reactions are also exothermic reactions with negative enthalpy change ($-\Delta H^{\circ}$).

Also included are four types of reduction reactions: Boudouard, the water-gas reaction, the water-gas shift reaction, and methane (CH_4) production (*See* Table 1, *reactions* 5 *to* 8). In a Boudouard reaction, Carbon dioxide (CO_2) reacts with carbon (C) to produce Carbon monoxide (CO). In a water-gas reaction, carbon (C) reacts with water (H_2O) to produce Carbon monoxide (CO) and Hydrogen (H_2). Both of these reactions are endothermic, resulting in positive enthalpy change ($+\Delta H^{\circ}$). The water-gas shift is a reaction of Carbon monoxide (CO) and water and produces Carbon dioxide (CO_2) and Hydrogen (H_2). Methane gas (CH_4) production results from a reaction between Carbon and Hydrogen (H_2).

3. Process simulation

The simulation of Jatropha shell was performed by an ASPEN PLUS package, a commercial software in energy process optimization for steady-state as shown in Fig. 3. It aims to estimate the composition of a product gas by calculating mass, energy balance, and chemical equilibrium of a process. ASPEN PLUS has many databases that include information about pure components as well as phase equilibrium data for conventional chemicals, electrolytes, solids and polymers. The user may provide additional data, such as the molecular weight, normal boiling point, specific gravity at 60 F (288 K), standard enthalpy and Gibbs energy formation. Because of the complexity of chemical structure, the coal and biomass stream used a category of 'non-conventional component'. Working with this component includes making proximate, ultimate, and sulphur analyses to calculate the enthalpy in the property methods.

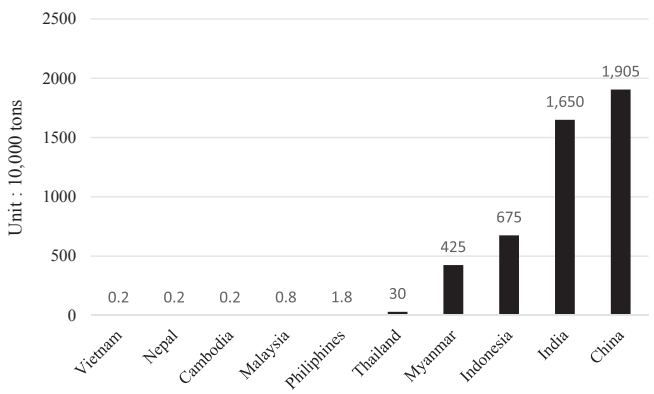

Fig. 1. Projection of *Jatrhopa curcas* production [20].

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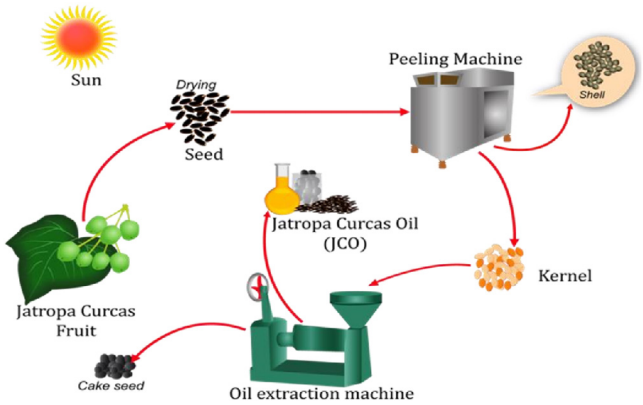

Fig. 2. The conversion of *Jatropha curcas Lynn* into crude Jatropha oil.

3.1. Block model

In ASPEN PLUS, blocks are placed into the flowsheet window and connected to each other by streams. Streams include material, heat and work, while block models include mixer, separator, heat exchanger, column, reactor, pressure changer, manipulator, solid and user models. In simulation, the blocks and streams are used to create a flowsheet. Drying and pyrolysis employ the RYIELD block, while oxidation and reduction employ a RGIBBS block as shown in Fig. 3.

The RYIELD block is used to decompose the non-conventional component into conventional components such as C, H, O and N. This process includes drying, which releases moisture (H_2O), and the pyrolysis process, in which the FEED breaks down into steam (H_2O), Carbon (C), Hydrogen (H_2), Nitrogen (N_2), Oxygen (O_2), Sulphur (S) and ash. The breakdown system is used because the block RGIBBS cannot perform the complex structure with a nonconventional component such as biomass. After the decomposition of FEED, the product yield (stream 1) is mixed with oxygen and nitrogen.

The RGIBBS block simulates both oxidation and reduction reactions by applying Gibbs free energy minimization in the system. The SEP block is then employed to simulate the separation process, removing gaseous product from carbon (C) and ash. ASPEN PLUS handles biomass as a nonconventional component, so no data for it is included in the software databanks. Therefore, the HCOALGEN model is used to calculate its heating value, heat capacity, heat of formation and heat of combustion.

Table 1
Chemical reaction in a gasifier (modified from [25]).

Reaction type	Reaction name	Chemical reaction	Enthalpy changes (ΔH°) (KJ/kmol)
Oxidation	1. Complete combustion	$C + O_2 \leftrightarrow CO_2$	−394
	2. Partial combustion	$C + ½\ O_2 \leftrightarrow CO$	−111
	3. Steam production	$H + ½\ O_2 \leftrightarrow H_2O$	−242
	4. CO oxidation	$CO + ½\ O_2 \leftrightarrow CO_2$	−283
Reduction	5. Boudouard reaction	$CO_2 + C \leftrightarrow 2CO$	+172
	6. Water-gas reaction	$C + H_2O \leftrightarrow CO + H_2$	+131
	7. Water gas shift reaction	$CO + H_2O \leftrightarrow CO_2 + H_2$	−42
	8. Methane production	$C + 2H_2 \leftrightarrow CH_4$	−75

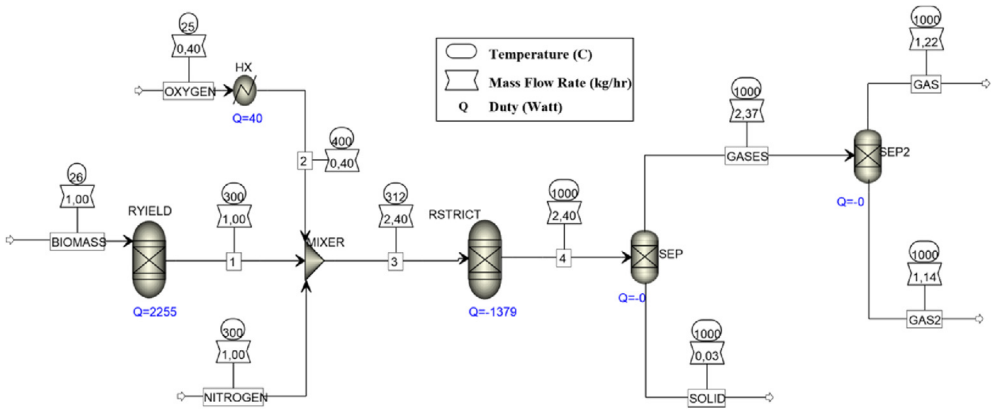

Fig. 3. ASPEN PLUS flowsheet model on gasification process.

3.2. Property method

The appropriate property method carries the correct composition of the product in a thermodynamics calculation. ASPEN PLUS uses data for enthalpy, density, temperature and heat duty and the specific property method to calculate the thermodynamic. For this research, the simulation uses Peng – Robinson property method because of its appropriateness for high temperature reactor models (e.g. entrained flow reactor models).

3.3. Feedstock data

The feedstock data for rice husk, sawdust, and Jatropha shell, including ultimate analysis for carbon (C), Hydrogen (H), Oxygen (O), Nitrogen (N), Sulfur (S) and Chlorine (Cl), as well as the data of proximate for moisture, ash volatile matter, and fixed carbon, are presented at Table 2. Based on the proximate data, Jatropha shell has high volatile matter at 65% and low at 3.8%, which may make it a good solid fuel for energy production. Furthermore, Jatropha shell has a proportion of 50.9% carbon, higher than sawdust at 48.99% and rice husk at 37.18%.

3.4. Model assumption

This simulation used several assumptions to build a model that is as realistic as possible. These include assuming steady state of the process, uniform temperatures in a bed, and char composed only of carbon (C) and ash. The RYIELD block was assumed for the drying and pyrolysis reaction, while oxidation and reduction reactions occur in RGIBBS. The SEP block was used to model a separation process with 100% efficiency of separation. The pyrolysis product was assumed by the equivalent elemental components.

3.5. Set-up of simulation data

Parameter data is needed for simulation with fixed and control variables as shown in Table 3. The temperature reactor is set between 1000 and 1400 °C and ambient pressure is set at 1.05 bar. The feedstock materials are rice husk and sawdust and have a feed flow rate of 1 kg/hr. Nitrogen (N_2) and oxygen are sent to the reactor at a temperature of 25 °C and with flow rates of 1 kg/hr and 0.4 kg/hr respectively.

3.6. Validation and mean error approach (MEA)

The simulations of rice husk and sawdust were used for validation alongside experimental data from Zhou et al. (2009) [31]. In this validation, some discrepancies appeared between data resulting from the experiment and the simulation because of the assumptions used in the simulation process. We calculated the errors proposed by Mansaray et al. [32] and applied it for the prediction of production from the Jatropha shell processes:

$$RSS = \sum_{i}^{N} \left(\frac{x_{i,e} - x_{i,sim}}{x_{ie}} \right)^2 \quad (1)$$

RSS is Residual sum of squares, N is total number of data points, $x_{i,e}$ is mol fractions of species i on experiment, and$x_{i,sim}$ is mol fraction of species i on simulation. RSS is created by the square value of the experimental data and simulation results in accordance with the number of data points taken. This is then divided by the number of data points, creating the mean value that is shown in Eq. (2).

$$MRSS = \frac{RSS}{N} \quad (2)$$

MRSS is Mean Residual Sum of Squares. It is calculated by dividing RSS by the total number of data points, N. Mean error itself is the result of root square of MRSS.

$$Mean\ error = \sqrt{MRSS} \quad (3)$$

4. Result and discussion

4.1. Validation of sawdust and rice husk

The first step of this research is to validate the common model with the experimental data of rice husk and sawdust which are presented in Figs. 4 and 5. The model is built in ASPEN PLUS simulation software.

Both the experiment and simulation use temperature as variable control with ranges from 1000 to 1400 C. Four species are compared: carbon monoxide (CO), carbon dioxide (CO_2), hydrogen (H_2), and methane (CH_4). The gas products obtained in the simulations are in agreement with the results of experiments for those four species. According to Le Chatelier's principle, higher temperatures favor products in endothermic reactions [33].

4.2. Jatropha shell gaseous products (Fiverr)

We then simulate the Jatropha shell in same model and presented the result in Fig. 5. Increasing the temperature of the reactor increases the production of carbon monoxide and hydrogen while decreasing the gaseous product of carbon dioxide and methane. However, the

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Table 2
The ultimate and proximate analysis of feedstock.

Material	Ultimate analysis (db wt %)						Ultimate analysis (db wt %)				HHV (MJ/kg)
	C	H	O	N	S	Cl	Moisture	Ash	Volatile	FC	
Rice husk [30]	37.18	4.26	31.29	0.8	0.15	0	9.23	17.21	58.69	14.87	18.279
Sawdust [30]	48.88	6.29	33.59	1.70	0.06	0	4.79	4.69	72.29	18.23	21.553
J. shell [31]	50.9	5.8	39.5	0.8	0.1	0.1	8.9	3.8	65	22.3	16.5

Table 3
The setup data is used by simulation.

Parameter	Value
Entrained flow reactor	
Temperature (°C)	1000–1400
Pressure (bar)	1.05
Feedstock material	
Rice husk (kg/h)	1
Sawdust (kg/h)	1
Nitrogen (N_2)	
Temperature (°C)	25
Flow rate (kg/h)	1
Oxygen	
Temperature (°C)	25
Flow rate (kg/h)	0.4
Preheater	
Temperature (°C)	400

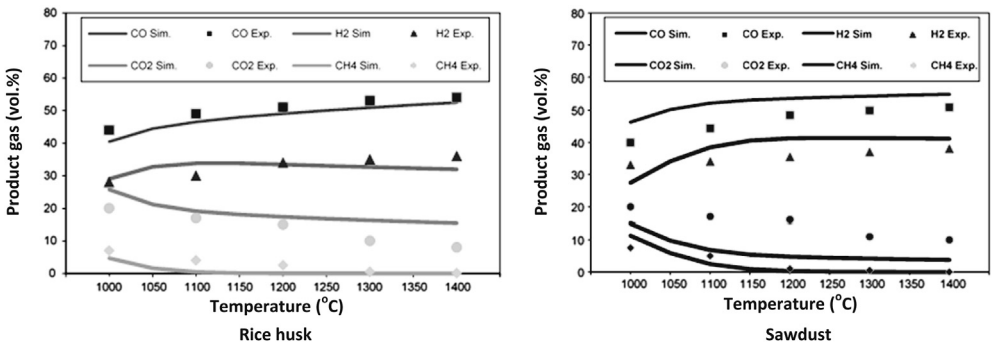

Fig. 4. Validation of rice husk and sawdust as a function of temperature.

gaseous product percentages are different. The gaseous product from Jatropha is always between that of sawdust and rice husk, suggesting that Jatropha shell can be a promising source of energy through gasification, as are sawdust and rice husk.

4.3. Mean error approach (MEA)

After data is obtained of simulation of Jatropha shell, we analyzed Mean Error value by MEA to understand the spread of the gaseous product. If this shell experimental data was available, this MEA would not have been necessary.

The result of the mean error approach is shown in Table 4. It can be seen that methane (CH_4) has the highest value both for sawdust and rice husk, meaning the gaseous products of methane (CH_4) were very different in the simulation and in the experiment. Carbon monoxide (CO) has the lowest value, indicating that the gaseous products of carbon monoxide (CO) in the simulation and experiment were similar.

4.4. Spread of Jatropha shell gases

Fig. 6 presents the spread of Jatropha shell gaseous product once the mean error approach is applied. The mean error approach provides information of the spread value of each substance, which then informs us of the maximum and minimum gaseous product of each substance. The stock chart is used to explain this spread and error values. In Fig. 6a, the prediction of carbon monoxide (CO) composition at temperatures of 1000 °C ranges from 40.54 to 52.32%. This means that after gasification of Jatropha shell at that temperature, carbon monoxide produced ranges from 45.54% at minimum or 52.32% at maximum. The other gaseous composition presented in Fig. 6b is hydrogen (H_2), with the result 27.07–35.91%. For carbon dioxide (CO_2), the minimum and maximum value of the gaseous product is 5.43–28.29% while for methane (CH_4) it is 0.49–9.96%.

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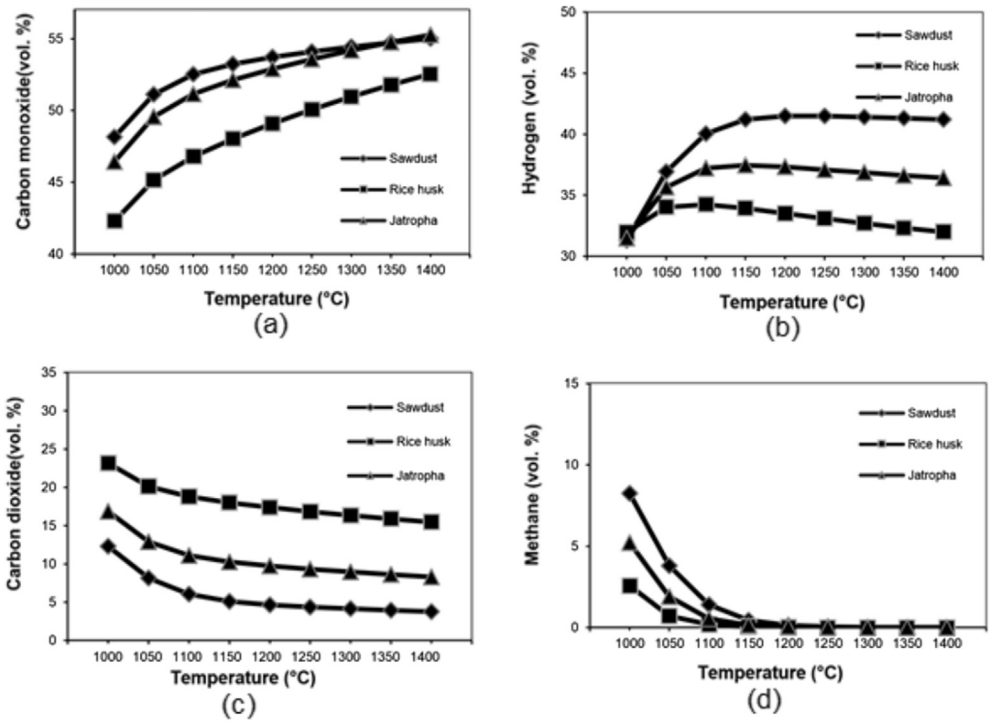

Fig. 5. The gaseous products result of Jatropha shell simulation compared with sawdust and rice husk (a) Carbon monoxide (CO), (b) Hydrogen (H_2), (c) Carbon dioxide (CO_2), (d) Methane (CH_4).

Table 4
Mean error value.

	Carbon monoxide (CO)	Hydrogen (H_2)	Carbon dioxide (CO_2)	Methane (CH_4)
Rice husk	0.0499	0.0838	0.5294	0.8776
Sawdust	0.1267	0.1367	0.5815	0.6115

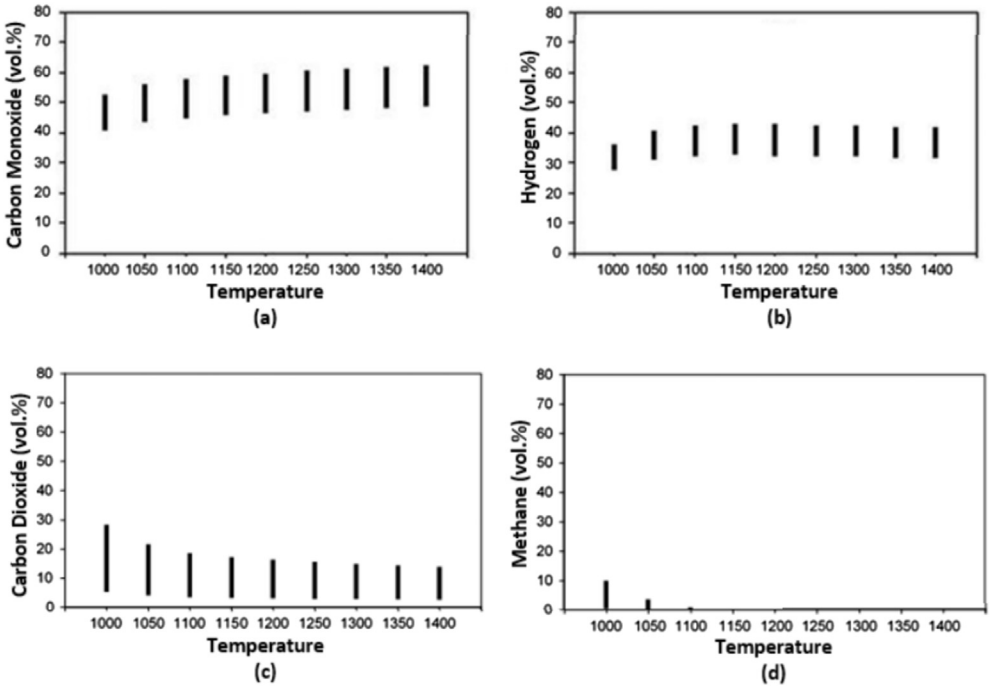

Fig. 6. Predictions of gaseous products according to mean error approach (MEA). (a) Carbon monoxide (CO), (b) Hydrogen (H_2), (c) Carbon dioxide (CO_2), (d) Methane (CH_4).

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5. Conclusion

Jatropha curcas Lynn is one of the biomass resources which are widely spread in several countries in the world. It is cultivated to produce biodiesel oil from it kernel. In the process of biodiesel oil production, it produces an abundant of by-products material such as shell and oil cake. In this research, Jatropha shell is utilized to produce energy through gasification with simulation. ASPEN PLUS commercial software has been used to simulate this gasification processes. Since there is no available data of Jatropha shell experiment, we validated the model using other biomass: rice husk and sawdust.

The validation results showed that the model agreed with the experimental data of rice husk and sawdust. Furthermore, the same model is applied for *Jatropha curcas* properties data. From this simulation, we obtained that carbon monoxide (CO) and hydrogen (H_2) increased when reactor temperature was raised. Meanwhile, carbon dioxide (CO_2) and methane (CH_4) decreased.

Since the simulation is not validated directly with Jatropha shell experimental data, error may come because of this situation. Therefore, we applied the Mean Error Approach (MEA) and produced a range of gas products through Jatropha shell in a simulation. The MEA data shows that methane (CH_4) has the highest mean errors with both sawdust and rice husk, at values of 0.8776 and 0.6115, respectively. Carbon monoxide (CO) on the other hand, has the lowest error. When we then apply this MEA to Jatropha shell simulation result, it shows that the range of carbon dioxide (CO_2) produced by Jatropha shell gasification has a composition ranging from 40.54 to 52.32% at a temperature of 1000 °C. The composition range of hydrogen (H_2), carbon dioxide (CO_2), and methane (CH_4) gases are 27.07–35.91%, 5.43–28.29%, and 0.49–9.96%, respectively.

More convergence is expected for the range of gaseous products in the simulation result of Jatropha shell once there is more experiment data to reference. However, if Jatropha shell experimental data were available for validation, the simulation result would be more accurate even without using the Mean Error Approach (MEA).

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