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COMPUTER-AIDED MODELLING OF THE PYROLYSIS OF RUBBER SAW DUST (*Hevea Brasiliensis*) USING ASPEN PLUS

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Abstract: Lignocellulosic biomass such as rubber (*Hevea brasiliensis*) saw dust is an energy-rich waste material that is readily available at local timber industries across Nigeria which can be sourced at very low or no cost. A steady-state sequential-modular simulation model was designed using ASPEN Plus V8.8 to evaluate the technical feasibility of applying pyrolysis technology for the recovery of energy from the biomass. The key pyrolysis parameters, such as the reaction temperature, pressure, flow rate and feeding rate were incorporated, and the product yields and properties was investigated and validated. The pyrolysis reactor was modelled by a combination of the RYIELD reactor and RGIBBS reactor. The model simulated the pyrolysis at 500°C and 1 atm to obtain a liquid yield of 58.9%. The Char and synthesis gas yield from the process were 18.7% and 22.4% respectively.

Keywords: Modelling, Rubber (*Hevea brasiliensis*) Saw Dust, Pyrolysis, Aspen Plus

INTRODUCTION

Forest and agricultural waste is a source of interest as an energy source. As a world average, about 15% of primary energy consumption is supplied from biomass and this figure rises to more than 35% when considering only developing countries (Cordero, Marquez, Rodriguez-Mirasol, & Rodriguez, 2001). Biomass is recognised as the third largest primary energy source in the world (Gani & Naruse, 2007). Lignocellulosic biomass such as rubber (*Hevea brasiliensis*) saw dust is a waste material that is readily available at local timber industries across Nigeria. It has a very rich carbon content and can be sourced at very low or no cost. Thermochemical processes are widely used for biomass conversion and energy recovery. These processes includes combustion, gasification, liquefaction, hydrogenation and pyrolysis (Goyal, Seal, & Saxena, 2008).

The products from the pyrolysis process are char, oil and gases and their distribution and composition are mainly dependent on temperature, heating rate and pressure (Di Blasi, Signorelli, Di Russo, & Rea, 1999). Fast pyrolysis can produce very good pyrolysis oil yields and contains up to 70% of the energy of the biomass feed (French & Czernik, 2010). However, certain bio-oil characteristics significantly hinder its widespread application. These properties include low heating value, incomplete volatility and acidity (French & Czernik, 2010). These undesirable properties of pyrolysis oil are as a result of an uncharacteristically high proportion of different classes of oxygenated organic compounds. Removing oxygen is thus necessary to reform the oil into an accepted and economically attractive fuel.

Fast pyrolysis for energy recovery has been carried out on numerous wood samples under different conditions to obtain good liquid yield (Prakash & Karunanithi, 2008), (Heo et al., 2010), (Gani & Naruse, 2007), (B. Peters & Bruch, 2003). Goyal et al.

(2008) in their extensive review presented pyrolysis products yield for an assortment of cellulosic and Lignocellulosic biomass samples. Sawdust samples that have been pyrolysed and reported includes Hinoki saw dust (Gani & Naruse, 2007), teak saw dust (Ismadji, Sudaryanto, Hartono, Setiawan, & Ayucitra, 2005), waste furniture saw dust (Heo et al., 2010), *Larix Leptolepis* saw dust (Park, Kim, Lee, & Lee, 2010), Pine saw dust (Oasmaa, Solantausta, Arpiainen, Kuoppala, & Sipilä, 2009) (Carlson, Cheng, Jae, & Huber, 2011), Red Oak and Sweet Gum saw dusts (Zhang, Toghiani, Mohan, Pittman, & Toghiani, 2007) and Douglas Fir saw dust (Ren et al., 2012).

Extensive work has been done to understand biomass pyrolysis in terms of kinetics and reaction sequence (Gavin, Stuart, & Emilio, 2016), (Srivastava & Jalan, 1996a, 1996b), (Alves & Figueiredo, 1989). Modelling and simulation of biomass pyrolysis (and gasification) using ASPEN Plus in particular (Yan & Zhang, 1999), (Tan & Zhong, 2010), (Samson, Shaharin, & Suzana, 2011), (Ramzan, Ashraf, Naveed, & Malik, 2011), (Abdelouahed et al., 2012), (J. F. Peters, Iribarren, & Dufour, 2013), (Ward, Rasul, & Bhuiya, 2014), (Onarheim, Solantausta, & Lehto, 2014) and other software in general (Zhang et al., 2007) have been explored.

Fast pyrolysis is a high temperature process in which biomass is rapidly heated an inert environment. Heating rate is somewhere about 300° C/min (Goyal et al., 2008). The biomass then vaporizes and condenses to a dark brown liquid known as pyrolysis oil. It has been observed that maximum yield of oil is obtained with high heating rates, at reaction temperatures around 500°C and short vapor residence times so as to minimize secondary reactions (Ward et al., 2014).

In the present study, simulation modelling of the pyrolysis rubber (*Hevea brasiliensis*) sawdust was

carried out with ASPEN Plus V8.8 to evaluate the technical feasibility of applying this technology to rubber sawdust. The key pyrolysis parameters, such as the reaction temperature, pressure, flow rate and feeding rate were incorporated, and the product yields and properties was investigated and validated.

METHODOLOGY

— Model component specification

In ASPEN Plus V8.8 the components are classified into major classes. In this research work, three component classes have been used: conventional components, non-conventional components and solids. In the global settings of the simulation, the stream class is set to MIXCINC as there are conventional and non-conventional solids alongside the conventional components. Particle size distribution will not be considered under this selection. Non-conventional components are not chemical components and they do not have a molecular formula. Instead, in Aspen Plus V8.8 they are specified by empirical factors representing their elemental composition. Enthalpy and density are the only properties calculated for non-conventional components and it is done by empirical correlations. The specific property methods for enthalpy and density for rubber wood were chosen as HCOALGEN method and DGOALIGT method respectively, which is based on ultimate analyses and proximate analyses. Rubber (*Hevea brasiliensis*) saw dust is a non-conventional material which is modelled in the ASPEN Plus by the proximate and ultimate analysis using the data in Table 1.

Table 1: Proximate and Ultimate Analysis of Rubber (*Hevea brasiliensis*) saw dust (Srinivasakannan & Bakar, 2004).

Proximate analysis (wt% wet basis)	
Moisture	6.20%
Fixed Carbon	23.38%
Volatile Matter	69.68%
Ash	0.74%
Ultimate analysis (wt% moisture free)	
Carbon	43.98%
Hydrogen	8.04%
Sulphur	0.45%
Oxygen	47.53%
Nitrogen	Nil

The conventional components added to the simulation include saturated aliphatic hydrocarbons C₁ – C₂₀. Nitrogen, Hydrogen Sulphide, some aromatic compounds and elemental carbon were the other components added to the simulation. Hydrogen Sulphide gas was added to the simulation to help account for the sulphur content of the biomass.

For the estimate the physical properties of the conventional components in the simulation, the Peng-Robinson with Boston-Mathias alpha function equation of state (PR-BM) was used. Alpha is a temperature dependent parameter that improves the

pure component vapor pressure correlation at very high temperatures (Altayeb, 2015). For this reason, PR-BM is suitable for the pyrolysis process since relatively high temperatures are involved.

— Reactor Model Description

The pyrolysis reactor was modelled in the simulation by two stages. The reactor was modelled by a combination of the RYIELD reactor and the RGIBBS reactor. The RYIELD (yield) reactor converts the dry non-conventional feedstock to conventional components. The RGIBBS (Gibbs) reactor calculates the final component distribution and phase equilibrium through the minimization of Gibbs free energy.

The Gibbs reactor in ASPEN Plus does not require a specified reaction stoichiometry. This reactor is suitable in simulating different types of chemical reactions amongst which is combustion, gasification and pyrolysis. Separation of the char from the vapour in the product stream is modelled by a cyclone. Reduction of product vapour temperature to induce condensation of liquid products is modelled by a heater set to ambient conditions.

Table 2: ASPEN Plus unit operations model description

ASPEN Plus ID	Block ID	Description
RYIELD	DECOMPOS	Conversion of non-conventional material (rubber saw dust) to conventional components
RGIBBS	PYRO	Calculation of the composition of the products through the minimisation of Gibbs free energy
SSPLIT	SEP1	Separation of the char from the product vapour by specifying split ratio
HEATER	CONDENSR	Condensation of the vapour products to give oil and non-condensable gases
FLASH2	SEP1	Separation of pyrolysis oil from non-condensable gases.

The following assumptions are considered in the simulation to reduce complexity. However, care was taken to prevent oversimplification of the model.

- ≡ The pyrolysis simulation model prepared with Aspen PLUS V8.8 is a steady-state isothermal model.
- ≡ All sulphur is represented as Hydrogen sulphide and char is assumed to be composed of elemental carbon alone.
- ≡ All elements take part in the chemical reaction except ash which is considered as inert.

— Process Model Description

A steady-state sequential-modular simulation model was designed using ASPEN Plus V8.8. Sequencing generally connotes designating the order of performance of tasks to assure optimal utilisation of available inputs (Licker, 2003). In ASPEN PLUS it connotes a sequential block-by-block calculation method where the results of one block serve as the basis for the next.

The simulation ambient temperature and pressure were specified as 25°C and 1 atm respectively. The saw dust (10kg/hr) and Nitrogen gas (0.1kmol/hr) was fed into the pyrolysis reactor block at ambient conditions. The Nitrogen helps to provide an inert environment in the reactor. The first reactor block converts the sawdust into conventional chemical components. The second reactor block predicts the final product distribution vis the minimisation of Gibbs free energy. The Nitrogen gas is specified as an inert in the Gibbs reactor.

The temperature and pressure of the reactor system is taken as the temperature and pressure of the final reactor block and they were specified at 500°C and atmospheric pressure. The process flow diagram (PFD) of the simulation is presented in Figure 1.

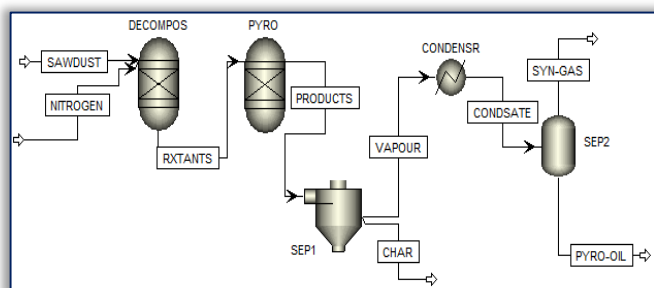


Figure 1: The process flow diagram (PFD) of the simulation

The cyclone is used to separate the char from the vapour products. The vapours are then condensed to ambient temperature before the final separation of the non-condensable gases from the oil. Due to the nitrogen gas present in the synthesis gas stream, actual synthesis gas amount will be estimated by subtracting the Nitrogen gas flowrate fed into the system from the overall gas flowrate.

RESULTS AND DISCUSSION

The results of the products yield at feed rate of 100kg/hr and 500°C pyrolysis temperature from the simulation are presented in Table 3.

Table 3: Results of Product Yields

Product	Yield (wt%)
Pyrolysis oil	58.90%
Char	18.70%
Synthesis Gas	22.40%

The results show a good yield of pyrolysis oil with respect to the other products. The synthesis gas and

char was composed of light hydrocarbons and elemental carbon respectively. The pyrolysis oil was composed of the other hydrocarbons and aromatics. Considering the technical and economic feasibility, rubber (*Hevea brasiliensis*) saw dust produces as good an oil yield as most other lignocellulosic feedstock available.

Pyrolysis of wood saw dust in general has been proved possible (Gani & Naruse, 2007; Heo et al., 2010; Ismadji et al., 2005; Oasmaa et al., 2009; Park et al., 2010) (Carlson et al., 2011; Ren et al., 2012; Zhang et al., 2007) and rubber (*Hevea brasiliensis*) saw dust is not be an exception. Financial/economic feasibility of biomass pyrolysis is still not as positive as expected. Wood pyrolysis is majorly justifiable from the standpoint of energy recovery from waste biomass and also that of environmental consideration. The oil itself still lacks full backing in the world market as it is generally considered as acidic and unstable (Perry H. Robert & Don, 1999).

Experimental data of the product composition from a pyrolysis process and the oil yield was used to validate the simulation model (Goyal et al., 2008). The product yield is fairly in line with experimental results for wood pyrolysis. There is a considerable difference between the simulation results and the experimental data with respect to product composition. Due to the extent of diversity of the components of pyrolytic oil, it is difficult to accurately quantify all of them.

The simulation model failed to evaluate the composition of the higher alkanes C₁₀ – C₂₀, and the concentrations of the other components are significantly varied from literature information. The reason behind these discrepancies is due to the Gibbs model calculating product compositions by minimizing Gibbs free energy as observed by other researchers (Altayeb, 2015).

In order to be able to obtain fairly accurate and reliable results consistent with the literature, a kinetic model based on reaction mechanisms needs to be established to predict the pyrolysis products with respect to biomass composition and operating factors. Considering that pyrolysis reactions stoichiometric relationships are still currently estimations, it is still quite difficult to obtain fully accurate results from the method.

CONCLUSION

A steady-state sequential-modular simulation model was designed using ASPEN Plus V8.8 to evaluate the technical feasibility of applying pyrolysis technology to rubber (*Hevea brasiliensis*) sawdust. The pyrolysis reactor was modelled by a combination of the RYIELD reactor and RGIBBS reactor.

The model simulated the pyrolysis at 500°C and 1 atm to obtain a liquid yield of 58.9%. The Char and synthesis gas yield from the process were 18.7% and 22.4% respectively.

The model showed correlation with literature in terms of product yield but not in terms of product composition. Discrepancies in compositional values were pinpointed on the inadequacy of the calculation technique utilised by the RGIBBS reactor.

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