Simulation of the gasification process of palm kernel shell using Aspen PLUS

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Abstract. This research sought to simulate gasification of palm kernel shell (PKS) in stationary state by using Aspen PLUS®. The model can predict the syngas composition with 1.6% absolute error. Biomass is defined as a non-conventional component from its proximate and ultimate analyses. The gasification process was divided into four stages: drying, pyrolysis, oxidation, and reduction, simulated in two R-Yield and R-Equil reactors, specified through the physicochemical characterization of the PKS and the chemical reactions in equilibrium intervening in the gasification. Simulation results were validated with experimental results from other investigations with similar operating conditions. Production of H2 and CO2 increases by increasing temperature from 700 to 900°C, contrary to what occurs with CO that diminishes at higher temperatures. The steam/biomass (S/B) ratio has a significant effect on the proportion of H2 in the syngas, given that it diminishes significantly by 20.3% upon increasing the S/B ratio from 1.5 to 2.5, showing the same trend for the CO and CO2 gases.

1. Introduction
Sustained increased use of fossil fuels, like coal, petroleum, and natural gas, has caused global energy dependence on non-renewable resources; this is evidenced in the current global primary energy supply for 2015, with 32% from petroleum, 28% from coal, and 22% from natural gas [1]. A global concern exists on the depletion of fossil resources, their high costs, negative environmental impacts within a scenario of increased energy consumption—a product of growing economies in each country [2]. Hence, many countries have focused their efforts on finding new energy sources that promote their energetic independence and solve said problem. In that sense, renewable energies have become the third greatest source in the global production of electricity, contributing 24.5% of the electric power in 2015 [3]. Approximately 50% of the electric power generated with renewable sources comes from hydroelectric plants, while only 6% comes from biomass [3]. Global energy trends show actions to develop and use so-called novel renewable energies (i.e., geothermal, solar, wind, tidal, and mini-hydraulic) in developed countries. In developing countries, for the rural population and the poorer zones in cities biomass is the only resource available to meet basic energy needs [4]. Therefore, these countries focus their efforts on developing and using biomass as renewable energy source due to its availability and low cost.
Biomass is recognized as an important renewable energy resource; its principal components include cellulose, hemicellulose, and lignin. Biomass sources for energy use are constituted by forest, livestock, industrial, agricultural, aquatic, and urban residues [5]. Some advantages of using biomass as energy resource are: its transformation into solid, liquid, or gaseous fuels; its energy use produces low toxic emissions and provides added value to residues considered wastes and even an environmental problem. Colombia has an important production of residual biomass, nearly 17.1 – million tons from the agricultural sector; some of the most important crops are sugarcane, oil palm, rice, corn, coffee, banana, and plantain, with an approximate capacity of 12,000MW/ year [6]. Of said biomass, the palm sector contributes 4.4%, comprised by empty fruit bunch (EFB), fiber, and palm kernel shell primarily [7]. Currently, part of the fiber and the PKS are used as solid fuel in boilers to produce steam and electric power, and EFB are used as fertilizers or soil conditioners, but long periods needed for their degradation can promote phytosanitary problems [5]. The remaining biomass is used in open areas, but due to its volume, it hinders its handling, without considering the environmental impact of the greenhouse gases that may be generated during its degradation process [8].

Industry has different processes for residual biomass use, like agrochemical, biochemical, and thermochemical processes. Among the latter, there is gasification, which is a process occurring in limited presence of oxygen combined with a carbonaceous material to produce a fuel gas comprised principally of H₂ and CO [9]. The process takes place in the presence of a gasifying agent (e.g., air, steam, oxygen), which depends on the type of gas sought, and it is conducted at temperatures ranging between 400 and 1500°C and at high atmospheric pressures (i.e., around 33 bar) [10]. The aim of this study was to model and simulate in Aspen PLUS® a fixed-bed gasifier in stationary state to predict the composition of the synthesis gas resulting from PKS gasification upon varying temperature and S/B ratio. Aspen PLUS® software permits managing solid components and has a broad chemical compounds database and a system to calculate the thermodynamic properties of the components and the chemical reactions [11]. Aspen PLUS® has been used by different authors to simulate thermochemical processes from biomass; thus, Mansaray et al., [12] used it to simulate rice husk gasification by using chemical equilibrium and energy balance ratios. Mathieu and Dubuisson [13] modelled wood gasification in a fluidized bed gasifier. Nikoo and Mahinpey [14] developed a model that predicts the yield of an atmospheric fluidized bed gasifier in stationary state, considering the hydrodynamics and reaction kinetics simultaneously.

2. Materials and methods

2.1. Palm biomass

The gasification process used palm kernel shell as raw material because of its vast availability and favorable physicochemical properties. In 2016, Colombia produced 302,573 tons of PKS [7]; currently, said material is used in extraction plants as boiler fuel. However, a large part of it is used in oil palm crops for roadway adaptation, thereby, leading to the energy waste of this material.

| Table 1. Characterization of the PKS [15]. |
|------------------------------------------|
| Proximate analysis (%) | Ultimate analysis (%) |
| M | A | VM | FC | CV | C | H | N | O | S |
| 7.52 | 2.67 | 69.35 | 20.46 | 18.96 | 46.05 | 5.14 | 0.62 | 45.40 | 0.14 |

M: Moisture, A: Ash, VM: Volatile matter, FC: Fixed carbon, CV: Calorific value (MJ/kg)

With respect to physicochemical characteristics, as evidenced in Table 1, PKS has high calorific value (18.96 MJ/kg), compared with other types of biomass, like sugarcane bagasse and rice husk with values of 15.11 and 14.09 MJ/kg, respectively [15]. Likewise, another important aspect is the low humidity content of PKS (7.52%) with respect to other raw materials, like coconut shell (18.50%), empty fruit bunch (66.26%) and sugarcane residues (52.20%) [16], making the gasification process more efficient because it does not require high energy consumption during the drying stage.
Additionally, Ng et al. [17] indicate that PKS has the highest hydrogen production (28.48 g H2/kg PKS) in the gasification process, compared with the sugarcane bagasse, rice husk, and coconut shell. Table 1 presents the proximate and ultimate analyses of the PKS, whose data will be subsequently input to the Aspen PLUS® for the specification of the non-conventional solid component.

2.2. Simulation in Aspen PLUS®

2.2.1. Assumptions. The following assumptions were considered in modelling the gasification process in Aspen PLUS®:
- Reactions occur isothermally and at constant volume.
- The gasification process takes place in stationary state.
- A homogenous mixture and temperature exist in the gasifier.
- The formation of tar and char is negligible and ignored in the gasification.
- The biomass particles are spherical and do not affect the reaction.

2.2.2. Gasification reactions. The method used in the simulation process in Aspen PLUS® is based on the Peng-Robinson equation of state, which permits estimating all the physical properties of the conventional components in stationary state. Its use improves the vapor pressure correlation of the pure components when temperature increases, such that its application is adequate to simulate the gasification process, where high temperatures are reached [18]. The gasification reactions shown in Table 2 are defined as reactions in chemical equilibrium and are incorporated in the OXI-RED reactor (Figure 1).

| Name of reaction          | Reaction           | Number |
|---------------------------|--------------------|--------|
| Incomplete oxidation      | C + 0.5O₂ → CO     | R-1    |
| Oxidation                 | C + O₂ → CO₂       | R-2    |
| Water gas                 | C + H₂O → CO + H₂  | R-3    |
| Boudouard                 | C + CO₂ → 2CO      | R-4    |
| Shift                     | CO + H₂O → CO₂ + H₂| R-5    |
| Hydrogasification         | C + 2H₂ → CH₄      | R-6    |
| Methanation               | CH₄ + H₂O → CO + 3H₂| R-7    |
| Ammonia formation         | N₂ + 3H₂ → 2NH₃    | R-8    |
| Hydrogen sulfide          | H₂ + S → H₂S       | R-9    |

2.2.3. Aspen PLUS® model. The gasification process was divided into four basic stages: drying, pyrolysis, oxidation, and reduction. Because the Aspen PLUS® does not handle a reactor that permits integrating all the stages, two reactors were used for modeling, bearing in mind different studies [19,20]. The first equipment is an R-Yield reactor fed with 10 kg/h of PKS, where the first phases take place and it is known as DRY-PYR in the gasification model (Figure 1); decomposition and devolatilization of the biomass are carried out in this equipment at 500°C and 1 bar pressure. The biomass introduced is fractioned into simpler components and converted from conventional to non-conventional components (e.g., H₂, CO, CO₂, CH₄, and H₂O). The yield of volatilization products is calculated in this reactor from the proximate and ultimate analyses of the PKS, without considering kinetics and stoichiometric reactions [19]. The reactor’s output current denominated DECOMP is mixed with steam in a mixer (MIX) at different S/B ratios (1.5 – 2.5) to determine its effect on the production of hydrogen (SYNGAS) present in the reactor’s output current. Said steam current (STEAM) is found at 150°C and 1 bar pressure to guarantee good-quality saturated vapor.

The second reactor integrates oxidation and reduction (OXI-RED) stages and consists of an R-Equil, based on a stoichiometric approach of the reactions in chemical equilibrium and does not require kinetic parameters for its specification. The MIX-GAS current from the mixer is fed to the OXI-RED reactor to carry out the reactions described in Table 2. This equipment operates at 1 bar pressure and at different
temperatures (700 – 900°C) to evaluate the effect of temperature on the hydrogen production in the reactor’s SYNGAS output current. Figure 1 shows the flow diagram of the gasification model developed in Aspen PLUS®.

![Flow diagram of the PKS gasification model.](image)

### Figure 1. Flow diagram of the PKS gasification model.

### 3. Results and discussion

#### 3.1. Model validation

Simulation results were validated through the experimental results from [21], which studied the gasification of residual palm biomass in a counter-flow fixed bed reactor. The present study analyzed the principal gases present in the syngas (H₂, CO, CO₂, CH₄) free of N₂ and in dry base, at 800°C and a S/B ratio of 1.5 (w/w). Table 3 shows the absolute error of each component, with a mean absolute error of 1.6%, from which a good level of fit is inferred of the simulated model with the experimental values. With respect to hydrogen current, when comparing the results of the model, with 2.1% error, with those obtained by [16], with 3.2% error, the goodness of fit of the model developed in this study is also noted.

#### Table 3. Analysis of simulated and experimental results.

| Type of gas | Sim. (% mol) | Exp. (% mol) | Abs. Error (%) |
|-------------|--------------|--------------|----------------|
| H₂          | 58.8         | 56.7         | 2.1            |
| CO          | 21.1         | 22.8         | 1.7            |
| CO₂         | 19.8         | 18.7         | 1.1            |
| CH₄         | 0.3          | 1.8          | 1.5            |

#### 3.2. Effect of temperature

In this case, the temperature effect was evaluated in the syngas production, especially in the hydrogen content; for this, temperature was increased from 700 to 900°C in the OXI-RED reactor at an S/B ratio of 2 (w/w), finding that increased temperature is directly proportional to hydrogen production (Figure 2(a)). In addition, the behavior of other gases, like CO and CO₂, was analyzed, determining that increased temperature promotes CO₂ production; on the contrary, CO production diminishes upon reaching 900°C (Figure 2(b)). The CH₄ content is not presented because it is < 0.5%.

This behavior is explained by addressing the Le Chatelier principle; high temperatures favor reagents in exothermic reactions and products in endothermic reactions [22]. Thus, increased temperature promoted the hydrocarbon endothermic reaction (R7), yielding increased H₂ concentration and a significant decrease in the CH₄ concentration. The CO was consumed mainly by the shift reaction (R5) to generate CO₂ and the increased temperature accelerated the reaction rate to produce CO₂. Hence, a decreasing trend is noted for CO with an increasing trend for CO₂. Turn et al., [23] found the same trend, likely attributed to high temperatures promoting thermal cracking of the hydrocarbon and reforming with steam. Asadullah et al., [24] and Lv et al., [25] also conducted biomass catalytic gasification studies, finding similar results in H₂ production, increasing at higher temperatures. However, regarding CO and CO₂, Asadullah et al., reported that CO content increased, while CO₂ content diminished after
the gasification reactor, while for Lv et al., the opposite was found. This difference can be attributed to the different reactors used in the modelling, operating conditions, and gasifying agents [22].

3.3. Effect of S/B ratio
Another variable evaluated in this study was the effect of the S/B ratio on the production of H₂, CO, CO₂; for this, a steam current was input into the mixer (MIX), as shown in Figure 1, at 150°C and 1 bar pressure. To guarantee the quality of the saturated vapor, the steam mass flow varied from 15 to 25 kg/h to maintain a 1.5 to 2.5 ratio between the steam and the biomass fed (10 kg/h of PKS). Figures 3(a) and 3(b) show that steam has an inversely proportional effect on the production of gases present in the output current of the OXI-RED reactor. No CH₄ production is registered, given that its value is < 0.1%

With respect to H₂ content, a decreasing trend is shown with increased S/B ratio from 1.5 to 2.5, explained by the input of an excessive amount of steam at a lower temperature than the internal temperature of the gasification reactor, causing a decrease in the reaction temperature and degrading the gas quality. This result resembles that occurring in [22], who obtained diminished H₂ production upon increasing the S/B range from 1.33 to 2.67 in the catalytic gasification of palm biomass. Furthermore, as shown in Figure 3(b), the CO and CO₂ content also revealed a decreasing trend upon increasing the S/B ratio from 1.5 to 2.5; this may be explained by more hydrocarbon steam reforming reactions (CO and CH₄) with increased amounts of steam [22].

4. Conclusions
The Aspen PLUS® software permits simulating the gasification of the PKS, given that it is possible to input the solid biomass as a non-conventional component from the proximate and ultimate analyses. The gasification process can be simulated in four stages: drying, pyrolysis, oxidation, and reduction, which occur industrially in a fixed bed counter-flow gasification reactor. These stages are carried out in R-Yield and R-Equil reactors, operating based on biomass yield and on chemical equilibrium reactions, respectively. The model can predict the yield of the PKS gasification process with a good level of fit
with the experimental results. Additionally, the sensitivity analysis in the software permits measuring the effect of the operating variables (temperature, S/B ratio) in the end product (H₂).

From the simulated results, it may be inferred that temperature has a directly proportional effect on hydrogen production; the opposite occurs for the S/B ratio, which has an inversely proportional effect on H₂ production. Upon increasing the temperature from 700 to 900°C in the OXI-RED reactor, the amount of H₂ in the syngas increases by 3.4%. However, upon varying the S/B ratio from 1.5 to 2.5 in the gasification process, H₂ production diminishes considerably by 20.3%; like gases, like CO and CO₂.

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