Numerical Studies on Fast Pyrolysis of Palm Kernel Shell in a Fluidized Bed Reactor

Thoharudin1,2, Yi-Shun Chen1 and Shu-San Hsiau1

1Graduate Institute of Energy Engineering, National Central University, Zhongli City, Taoyuan County, 32001, Taiwan ROC
2Department of Mechanical Engineering, Universitas Muhammadiyah Yogyakarta, Jl. Brawijaya, Kasihan, Bantul, D.I. Yogyakarta, Indonesia

Email: thoharudin@ft.umy.ac.id

Abstract. Numerical studies using Computational Fluid Dynamics (CFD) of thermal decomposition of Palm Kernel Shell (PKS) have been conducted in a fluidized bed reactor under atmospheric pressure of nitrogen as fluidization gas. To investigate the effect of temperature, the fast pyrolysis temperature was varied in a range from 400 °C to 650 °C. Furthermore, the effect of PKS feeding rate was also studied in a range from 300 g/h to 1500 g/h combined with variations of nitrogen superficial velocities. It was found that the increase of temperature results in the greatening of conversion efficiency and non-condensable gas product yield. The maximum 60.5 % liquid/tar product yield was obtained in 500 °C. The increase of PKS feeding rate led to the reduction of conversion efficiency due to the thermal energy shortage for the decomposition process. However, the increase of PKS feeding rate could reduce the non-condensable gas product with the insignificant change in liquid product yield. The rising superficial velocity of nitrogen favoured the shorter residence time resulting in the increasing tar product yield.

1. Introduction

Palm Kernel Shell (PKS) is abundant biomass residue derived from palm oil production which has a potential resource of renewable energy in Indonesia. In 2015, Indonesia had 8.4 million tons of PKS solid residue which has high carbon content currently used as combustion fuel with very limited efficiency [1]. A promising technology to convert solid biomass into liquid fuel, a useful form of energy, is pyrolysis. Pyrolysis is thermal decomposition of biomass in the absence of oxygen to produce liquid bio-fuel, bio-char and non-condensable gas products. An advanced pyrolysis technology, called as fast pyrolysis, involves fast heating rate and short residence time in medium temperature to maximize the liquid product [2].

Fluidized bed reactor is a popular, widely used and the most successful fast pyrolysis reactor due to many advantages, such as it has continue operational system, simple design and easy scale-up. Moreover, fluidized bed reactor offers a good solid mixing which enables biomass decompose rapidly because of the large surface contact between biomass and bed material as a heat transfer medium. In addition, fluidized bed reactor also provides a short residence time by controlling the fluidization gas flow rate to minimize the secondary cracking of tar which forms non-condensable gas product (NCG) [3].

Pyrolysis of PKS is very attractive to be investigated. High lignin content in PKS makes its bio-oil rich of phenol compound as reported in previous study [4]. Phenol is derived from rich-carbon lignin (Lign-C) and hydroxyl-rich lignin (Lign-OH) decomposed into sinapaldehyde or lumped phenol compound ($C_{11}H_{12}O_4$). Lign-C decomposes into Lign-CC, phenol and other compounds. Moreover,
Lign-CC degrades into phenol and other compounds including char and NCG. In other hand, Lign-OH degrades into lignin and other chemicals, and furthermore lignin decomposes into phenolic compound [5]. The advantage of phenol-rich bio-oil does not only serve as bio-fuel but also shows a great potential source to replace fossil phenols as high-valued chemicals feedstock such as cosmetic, food aromas, resins, pharmaceuticals, pesticides, and etc. currently produced from petrochemical feed stocks extracted from non-renewable resources [6], [7].

Computational fluid dynamics (CFD) is widely used to predict and analyze the phenomena in thermal decomposition process including pyrolysis. Aramideh, et al. [8] conducted numerical study to investigate the productivity of fast pyrolysis using an auger reactor. Jalalifar, et al. [9] investigated numerically the operating factors influencing on the pyrolysis product yields of common biomass pyrolysis in a bubbling fluidized bed reactor. Borello, et al. [10] simulated pyrolysis of sawdust in a packed bed reactor. There are many pyrolysis kinetic schemes provided in the literatures [5], [11], [12]. However, the global kinetic scheme offers a sufficient accurate prediction and simplicity in the use. Therefore, this study aims to investigate numerically the productivity of PKS pyrolysis in a fluidized bed reactor using global kinetic scheme.

2. Methods
A combination of laminar Multi-Fluid Model (MFM) and a chemical kinetic stiff heterogeneous reaction were taken into account using conservation laws of mass, momentum, energy, and species in Eulerian-Granular approach. In general, MFM consists of one gas phase as the primary phase and numbers of solid phases as the secondary phases. These models were solved using a commercial ANSYS Fluent CFD code. In this work, two solid phases were employed, namely biomass and sand. The gas phase consisted of three species, namely tar, non-condensable gas (NCG) and nitrogen. Meanwhile, the biomass phase comprised of nine species, namely cellulose, hemicellulose, lignin, active cellulose, active hemicellulose, active lignin, cellulose char, hemicellulose char, and lignin char. Sand as a bed medium consisted of one species and did not involve in the chemical reaction.

![Global kinetic scheme of pyrolysis](image)

**Table 1. Parameters of pyrolysis global kinetic scheme**

| Component | Reaction | Y of k | A (s^{-1}) | E (MJ.kmol^{-1}) | ΔH (kJ.kg^{-1}) |
|-----------|----------|--------|------------|-----------------|----------------|
| Cellulose | k_{1,c}  | -      | 2.8 x 10^{19} | 242.4           | 0              |
|           | k_{2,c}  | -      | 3.28 x 10^{14} | 196.5           | 255            |
|           | k_{3,c}  | 0.35   | 1.3 x 10^{10}  | 150.5           | -20            |
|           | k_{1,h}  | -      | 2.1 x 10^{16}  | 186.7           | 0              |
| Hemicellulose | k_{2,h} | -      | 8.75 x 10^{15} | 202.4           | 255            |
|           | k_{3,h}  | 0.6    | 2.6 x 10^{11}  | 145.7           | -20            |
|           | k_{1,l}  | -      | 9.6 x 10^{6}   | 107.6           | 0              |
| Lignin    | k_{2,l}  | -      | 1.5 x 10^{9}   | 143.8           | 255            |
|           | k_{3,l}  | 0.75   | 7.7 x 10^{6}   | 111.4           | -20            |
| Tar       | k_{4}    | -      | 4.28 x 10^{6}  | 108.0           | -42            |

A global kinetic scheme was considered to solve the pyrolysis simulation. Biomass in a single particle comprised of cellulose, hemicellulose, and lignin, transforms into active biomass by absorbing thermal energy provided by preheated nitrogen and heat source locating along the heater wall. Then, active biomass decomposes into tar, NCG and char. Furthermore, tar degrades into NCG as the consequence of secondary cracking reaction (k4). The reaction scheme and its kinetic parameters are...
described in Fig. 1 and Table 1 [13], respectively. All reactions are expressed using an Arrhenius form as given in equation 1.

\[ k_i = A_i \cdot \exp \left( \frac{-E_i}{RT} \right) \]  

(1)

Where \( k_i \) is the kinetic constant of reaction rate, \( A_i \) denotes the Arrhenius pre-exponential constant and \( E_i \) represents the activation energy of the chemical reaction. \( R \) and \( T \) indicate the universal ideal gas constant and temperature, respectively.

The sketch of fluidized bed reactor geometry is illustrated in Fig. 2 which accords to the work conducted by Xue, et al. [14]. 2-D simulations were used to perform the numerical studies due to its low computational cost and a relatively accurate result compared to 3-D simulation [14]. Biomass consisted of cellulose, hemicellulose, and lignin was injected into the reactor at 300 g/h of mass feeding rate and conditioned at 27 °C. A 0.4 mm constant particle diameter of biomass was used in all of the simulations. Pure nitrogen as fluidization gas was preheated until 500 °C and flowed from the bottom of the reactor at a superficial velocity of 0.36 m/s. An electric heater as a thermal energy source was performed as a constant temperature wall maintained at 523 °C. Silica sand employed as a bed medium had a diameter of 0.52 mm, initially heated to 500 °C and packed to a height of 55 mm with a volume fraction of 0.59. The initial sand temperature was set at the same temperature with the preheated nitrogen.

The simulation results were compared to the experiment reported by Xue, et al. [14] that used red oak as biomass raw material for pyrolysis in a fluidized bed reactor. Read oak consists of cellulose, hemicellulose, and lignin in the composition ratio of 0.41, 0.32 and 0.27 respectively. This work used PKS as the raw material which has 0.296, 0.232 and 0.472 of cellulose, hemicellulose and lignin, respectively, adapted from a study reported by Abinsa, et al. [15] by neglecting the extractive composition.

The velocity inlet was used as a boundary condition in biomass and preheated nitrogen inlets. One atmospheric pressure was used at the pressure outlet. A no-slip boundary condition was applied to heater wall and adiabatic wall for gas phase and 0.05 of specularity coefficient was implemented for solid phases to both types of wall adopted from Dinh, et al. [16]. Thermo-physical properties of species contributed in the pyrolysis are listed in Table 2 [17].
The conservation equations were solved using the phase coupled SIMPLE algorithm for the pressure-velocity coupling and the least square cell-based was applied to the pressure based solver. The equations of momentum and energy were calculated using the second order upwind, while the species equation was estimated using the first order upwind method. The volume fraction was discretized using the QUICK algorithm. The first-order implicit scheme for transient formulation was applied with the time step size of $1.25 \times 10^{-4}$ s to $5.0 \times 10^{-4}$ s, depending on the iteration stability. The simulations were performed for a reaction time of 30 s. The yields of the products (tar, NCG, char, residue) and the conversion efficiency were calculated using equation 2 to 6.

| Phase          | Species          | Molar Mass (kg.kmol$^{-1}$) | Particle diameter (mm) | Density (kg.m$^{-3}$) | Specific heat (J.kg$^{-1}$.K$^{-1}$) | Dynamic viscosity (kg.m$^{-1}$.s$^{-1}$) | Thermal conductivity (W.m$^{-1}$.K$^{-1}$) |
|----------------|------------------|------------------------------|------------------------|-----------------------|--------------------------------------|------------------------------------------|------------------------------------------|
| Gas            | Nitrogen         | 28                           | -                      | -                     | 1121                                 | $3.58 \times 10^{-5}$                    | $5.63 \times 10^{-2}$                    |
|                | NCG              | 30                           | -                      | -                     | 1100                                 | $3.0 \times 10^{-5}$                     | $2.577 \times 10^{-2}$                   |
|                | Tar              | 100                          | -                      | -                     | 2500                                 | $3.0 \times 10^{-5}$                     | $2.577 \times 10^{-2}$                   |
|                | Cellulose        | 162                          |                        |                       |                                       |                                          |                                          |
| Biomass        | Hemicellulose    | 132                          | 0.4                    | 400                   | 2300                                 |                                          |                                          |
|                | Lignin           | 208                          |                        |                       |                                       |                                          |                                          |
|                | Cellulose char   | 12                           |                        |                       |                                       |                                          |                                          |
| Char           | Hemicellulose char | 12                          | 0.4                    | 2333                  | 1100                                 |                                          |                                          |
|                | Lignin char      | 12                           |                        |                       |                                       |                                          |                                          |
| Sand           | Silica           | 60                           | 0.52                   | 2649                  | 800                                  |                                          |                                          |

\[
Y_i = \frac{m_i}{m_{biomass}} \quad (2)
\]

\[
\eta_{conversion} = 1 - Y_{residue} \quad (3)
\]

Where $Y_i$ indicates the yield of product species (tar, NCG, char, and residue), $m_i$ is the total mass of the product species including the product which still remains in the reactor and $\eta_{conversion}$ represents the conversion efficiency.

### 3. Results and Discussions

#### 3.1. Validation Data

The simulation results using red oak as biomass pyrolysis raw material was compared to the experimental data given by Xue, et al. [14], presented in Table 3. The results showed a good relationship between the simulation and experimental red oak pyrolysis data by comparing the product yields distribution and those relative different. Both experiment and simulation product yields of fast pyrolysis were dominated by tar product and followed by NCG and char products with relative differences of 9.7 %, 0.1%, and 17.2%, respectively. Therefore, the simulation model showed a promising capability to investigate different type of biomass (PKS in this work).

Table 3 also shows the comparison between red oak and PKS pyrolysis that indicates pyrolysis of PKS produces a larger amount of char product with the lower products of tar and NCG. It is well known that the composition of biomass has a significant impact on the yields of pyrolysis product. The phenomenon is attributed to the lignin decomposition characteristic. Lumped kinetic scheme reported by Ranzì, et al [5] explained the detailed decomposition of lignin which produces more char compared to cellulose and hemicellulose.
### Table 3. Comparison of product yields

| Method    | Biomass            | Tar (%)  | NCG (%) | Char (%) | Residue (%) | Ref.       |
|-----------|--------------------|----------|---------|----------|-------------|------------|
| Experiment| Red Oak            | 71.7 ± 1.4 | 20.5 ± 1.3 | 13.0 ± 1.5 | -           | [14]       |
| Simulation| Red Oak            | 64.8     | 18.6    | 10.8     | 5.9         | This work  |
| Simulation| Palm Kernel Shell  | 57.4     | 17.2    | 19.3     | 5.7         | This work  |

In this work, PKS was used as the raw material in fast pyrolysis in a fluidized bed reactor. The tar, NCG, and char product yields were 60.5%, 18.0%, and 16.6%, respectively. Compared to the study by Abnisa, et al. [15] which reported that the tar, NCG and char product yields were 47.43%, 17.31%, and 35.26%, respectively. Our work showed higher tar product with the lower char product. This difference was caused by the PKS particle size and the heating rate, whereas our work used smaller particle size and larger heating rate that contributed to the large amount of tar product with the low char product.

### 3.2. Effect of Fluidizing Gas Temperature

Operating temperature is an essential parameter for the kinetic rate of pyrolysis and it influences the chemical conversion efficiency and its product yields. Biomass consists of cellulose, hemicellulose, and lignin, which have a different characteristic in the decomposition process. Hemicellulose decomposes in a temperature range of 150 to 350 °C, while cellulose degrades at higher temperature ranges, namely 275-350 °C. In the other hand, lignin is a biomass constituent which has the highest temperature decomposition. The decomposition begins at a temperature of 280 °C and it reaches a peak rate at 350-450 °C [18]. PKS is dominated by lignin constituent that strongly influences the conversion efficiency. The higher temperature resulted the elevating conversion efficiency of biomass pyrolysis as presented in Fig. 3. The gradient of conversion efficiency increased sharply in the temperature range of 400 to 500 °C then followed by insignificant increasing conversion at the temperature above 500 °C. The high content of lignin in PKS contributes to the difficulty of PKS to be decomposed. Therefore, PKS needs medium-high temperature to maximize the decomposition efficiency.

Fig. 3 also provides the product yields distribution. The increasing temperature until 500 °C led the greatening of tar, NCG and char products with the decrease of residue or unreacted biomass. Furthermore, the increase of temperature above 500 °C caused to the rising of NCG product significantly with the decrease of tar and char products. High temperature promoted the secondary cracking reaction that converts tar into NCG, therefore the tar product decreases drastically at the temperature above 500 °C. The maximum tar product yield was obtained at 500 °C.

### 3.3. Effect of PKS feeding Rate

Pyrolysis is a thermal decomposition which means the process needs thermal energy input to carry out the decomposition. Thermal energy not only for heating the biomass, but also it is needed to perform the chemical conversion process. The biomass feeding rate is one of the important parameters that influence the thermal decomposition process. Greater feeding rate of biomass required higher thermal energy input to support the process. Therefore, the increasing feeding rate induced the decreasing temperature inside the reactor due to insufficient thermal energy input as illustrated in Fig. 4. All variations of feeding rate were flowed with 0.36 m/s of nitrogen as fluidizing gas at 500 °C from the bottom side of the reactor. The increasing feeding rates from 300 g/h to 1500 g/h caused the decrement of average reactor temperature from 500 °C to around 400 °C.

The decreasing temperature inside the reactor induced the increasing of both surface heat flux and surface heat transfer coefficient due to the larger temperature difference between the heater wall and biomass as presented in Fig. 5. This phenomenon indicates that the thermal energy input for the decomposition process increased with the raising of PKS feeding rates. Nevertheless, the elevation of thermal energy input into the reactor was still insufficient to maintain the reactor temperature well so that the temperature dropped significantly. As the consequence, the product yields distribution changed associated with the average operating temperature inside the reactor as shown in Fig. 6.
Fig. 6 shows the relationship between PKS feeding rates toward the pyrolysis product yields and its conversion efficiency. The increases of PKS feeding rate contributed to the decreases of conversion efficiency indicated by the rising of unreacted PKS as residue. The temperature drop due to insufficient energy input reduced the decomposition rates which favors the decrement of conversion efficiency and char product. In addition, the greater PKS feeding rates resulted in the decrease of tar and NCG product yields. The decrement was attributed to the lowering the primary decomposition rate of PKS due to the temperature drop inside the reactor.

![Figure 4](image)

**Figure 4.** (a) Biomass temperature contour inside the reactor (b) Biomass temperature distribution in the centerline of reactor.

![Figure 5](image)

**Figure 5.** Surface heat flux and surface heat transfer coefficient of heater wall.

![Figure 6](image)

**Figure 6.** Product yields of PKS pyrolysis for different PKS feeding rates.

### 3.4. Effect of Fluidizing Gas Superficial Velocity

Nitrogen as fluidizing gas in fluidized bed reactor performs as a heat carrier in the decomposition process, controls the volatile vapour residence time and it has a responsibility to the mixing/segregation between biomass and bed material. Larger superficial velocity of nitrogen indicates the greater energy supply for pyrolysis, shorter residence time, and more rapid mixing between PKS and bed material. Consequently, biomass decomposes rapidly due to the increase of biomass particle heating rate and the tar product elevates due to the minimum rate of secondary cracking reaction. This phenomenon is presented in Fig. 7. The increase of superficial velocity of nitrogen induced to the rising of tar product with the lowering of residue, whereas the char and NCG products showed the insignificant changes in all of feeding rate variations. The superficial velocities of nitrogen were varied i.e. 0.36 m/s, 0.55 m/s, and 0.75 m/s with the estimated residence time of 0.95 s, 0.62 s, and 0.46 s respectively.
Fig. 7 also shows the PKS pyrolysis product yields on the three variations of feeding rates. Those three variations demonstrated the increase of tar product by the elevating nitrogen superficial velocity, whereas the NCG product exhibited insignificant changes. The prominent phenomenon was shown in the residue product where the feeding rates of 1000 g/h and 1500 g/h displaying the drastic decrement with the raising of nitrogen superficial velocity. It also indicates that the increase of fluidizing gas velocity induced the elevating conversion efficiency. This was caused by the energy supply of preheated nitrogen that tends to be used for the primary decomposition rather than secondary cracking reaction resulting a sharp decline in residue product with a slight decrease in NCG product. Because pyrolysis has successive and competitive reactions, the product yields of pyrolysis are influenced by many parameters. Therefore, with the accordant parameters such as medium temperature, appropriate biomass feeding rate and nitrogen superficial velocity, the optimum tar product yield can be achieved.

4. Conclusion

In this present study, the global kinetic scheme approach was used to conduct the numerical studies of PKS pyrolysis. Compared to the red oak, pyrolysis of PKS produced larger char product yield with lower tar product yield due to its deferential biomass properties (percentage of cellulose, hemicellulose, and lignin). The increases of nitrogen temperature until 500 oC led to the increases of tar product, while at the above temperature, tar product decreased significantly due to the secondary cracking effect. Therefore, the maximum tar product could be attained in medium temperature (500 °C). The larger PKS feeding rates made the reactor temperature drop that induced the decomposition rate to become low so that the residue/unreacted biomass increased. However, by raising the nitrogen superficial velocity, the residue decreased with the tar product elevated due to bigger thermal energy input from preheated nitrogen even though in a large PKS feeding rate. Therefore, the PKS feeding rate and nitrogen superficial velocity should be maintained in order to achieve the appropriate temperature distribution along the reactor so that the optimum tar product yield could be attained.

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