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Process Simulation of Oil Palm Empty Fruit Bunch (OPEFB) Pyrolysis using Open-Source DWSIM: Analysis of Temperature-Dependent Product Yields

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Abstract

This study investigates the pyrolysis of Oil Palm Empty Fruit Bunches (OPEFB) using the open-source process simulation software DWSIM to evaluate the impact of temperature on product distribution, particularly bio-oil, biochar, and pyrolysis gas. OPEFB, an abundant lignocellulosic waste from Indonesia's palm oil industry, holds significant potential as a renewable biomass feedstock. The simulation model was developed based on thermochemical conversion principles and was validated against selected experimental data from the literature. Results show that pyrolysis temperature significantly influences the yield and composition of the products. The gas yield increased with temperature up to 460°C, dominated by CO, CO_2, and H_2 due to the decomposition of volatile organic matter. However, gas yield declined beyond 460°C, likely due to secondary reactions converting gas precursors into liquid products. The optimal temperature was found to be around 510°C, offering a balanced yield of bio-oil and gas with minimal biochar formation. The chemical composition of bio-oil included furfural, phenols, alcohols, and acetic acid—compounds derived from the breakdown of cellulose, hemicellulose, and lignin. Biochar yield decreased with temperature, but its quality improved in terms of carbon content and fixed carbon fraction. This study highlights the utility of DWSIM as an accessible and transparent tool for simulating biomass pyrolysis. Future work should focus on refining the kinetic parameters, experimental validation of simulation results, and integrating downstream processing for fuel and chemical recovery.

INTRODUCTION

Palm oil-producing countries, particularly Malaysia and Indonesia, are increasingly focusing on the utilization of biomass due to its environmental and economic benefits (Papilo et al., 2022). Among the byproducts of palm oil production, oil palm empty fruit bunches (OPEFB) represent a significant and underutilized lignocellulosic biomass (Haryanto et al., 2021). Effective valorization of OPEFB has the potential to reduce environmental pollution, mitigate greenhouse gas emissions, and create value-added products that support the circular bioeconomy. Several studies have demonstrated that converting palm biomass residues such as OPEFB, palm kernel shells, and mesocarp fiber into biofuels and biochemicals results in net negative carbon emissions (Beaudry et al., 2018; Norrrahim et al., 2022; Obada et al., 2023).

OPEFB is particularly attractive for thermochemical conversion due to its high volatile matter content, low ash, and low nitrogen and sulfur levels (Nyakuma et al., 2015). It contains cellulose, hemicellulose, and lignin, which are ideal precursors for producing energy-rich products via

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pyrolysis. Thermogravimetric analysis (TGA) indicates that OPEFB undergoes significant mass loss during pyrolysis, suggesting high conversion efficiency (Ahmad et al., 2025). Depending on the pyrolysis conditions, OPEFB can yield various products: slow pyrolysis (≤300 °C) favors biochar production with applications in soil remediation and wastewater treatment, while fast pyrolysis (450–500 °C) maximizes bio-oil yield with potential use as an alternative fuel (Rosli et al., 2017).

Despite these advantages, optimizing pyrolysis to control product distribution remains a technical challenge. Pyrolysis temperature is a critical parameter that governs the yield and quality of biochar, bio-oil, and syngas (Sekar et al., 2021). Numerous studies confirm that increasing pyrolysis temperature enhances gas production while reducing char yield (Bai et al., 2020). Therefore, understanding the thermal behavior of OPEFB during pyrolysis is essential to improve efficiency and tailor product outputs.

In this context, process simulation serves as a powerful tool for evaluating and optimizing pyrolysis operations without the need for costly experimental trials. While commercial software like Aspen Plus and ChemCAD are widely used, their high cost can limit accessibility for researchers and small enterprises. DWSIM, an open-source process simulator, offers a viable alternative with capabilities for modeling heat and mass transfer, chemical reactions, and phase equilibrium (Ullah et al., 2025). Its accuracy has been validated in previous studies, with simulation results showing minimal deviation from those of commercial platforms (Andreasen, 2022a).

However, limited research has focused on simulating OPEFB pyrolysis using open-source platforms such as DWSIM. Most existing simulation studies rely on commercial software, leaving a significant gap in accessible, low-cost modeling tools for biomass conversion processes. Moreover, few studies have systematically investigated the effect of operating temperature on pyrolysis product distribution using simulation-based approaches.

This study addresses this gap by developing a process model of OPEFB pyrolysis in DWSIM to investigate the effect of operating temperature on the distribution of biochar, bio-oil, and gas products. The novelty of this work lies in the application of a free and open-source simulation platform for modeling biomass pyrolysis, enabling broader access to advanced process design tools. The findings provide insights into temperature-dependent behavior of OPEFB during pyrolysis and demonstrate the utility of DWSIM for thermochemical process simulation in sustainable biomass valorization.

METHODS

Feedstock Characterization

OPEFB are a major lignocellulosic by-product of the palm oil industry. They consist predominantly of three structural biopolymers: cellulose, hemicellulose, and lignin. According to Rosli (2017), cellulose constitutes approximately 31.2% to 46% of the total dry weight of OPEFB, making it the most abundant component. Hemicellulose content ranges from 18.7% to 34%, with xylan identified as the primary polysaccharide, which can be hydrolyzed into xylose. Lignin accounts for about 20% to 27.7% of OPEFB and plays a critical role in providing mechanical strength and structural integrity to plant cell walls.
For this study, the compositional data reported by Hidayah and Wusko (2020) were adopted as the feedstock basis for the DWSIM simulation. The composition used includes 55.75% cellulose, 15.32% hemicellulose, and 28.93% lignin by weight. In the simulation model, cellulose was represented by its monomer unit, glucose, while hemicellulose was modelled using its dominant monomer, xylose. Lignin was assumed to behave as kraft lignin, a common representative model in thermochemical simulations. The elemental (ultimate) and proximate analysis data of OPEFB, required for estimating thermophysical and reaction parameters, were obtained from the previous study by Kusworo et al. (2020) and are summarized in Table 1.

Process Description

Biomass pyrolysis is a thermochemical conversion process that involves the thermal decomposition of organic material in the absence of oxygen, resulting in the formation of three primary products: solid biochar, liquid bio-oil, and non-condensable gases (Chormare et al., 2023). This process is considered a promising route for converting lignocellulosic biomass into renewable fuels and chemicals, supporting both waste

Table 1. Ultimate and proximate analysis of OPEFB (Kusworo et al., 2020).

Parameters	Unit	value
Carbon (C)	wt.%	42.32
Hydrogen (H)	wt.%	5.74
Nitrogen (N)	wt.%	1.84
Sulfur (S)	wt.%	0.26
Oxygen (O)	wt.%	39.24
Moisture	wt.%	9.20
Volatile matter	wt.%	61.00
Fixed carbon	wt.%	19.20
Ash content	wt.%	10.60
Higher heating value	MJ/kg	16.78

valorization and sustainable energy production. The pyrolysis process typically consists of three main stages: drying, thermal decomposition, and product separation (Devi et al., 2021). The drying stage is essential for reducing the moisture content of the feedstock, as high moisture levels can adversely affect heat transfer, energy efficiency, and product quality (EL-Mesery & El-khawaga, 2022). Effective moisture removal prior to pyrolysis enhances thermal conversion and reduces the energy required during processing.

The core of the pyrolysis process takes place in the reactor, where the feedstock is heated to elevated temperature typically in the range of 300°C to 700°C under inert or oxygen-limited conditions (Do & Nguyen, 2024). During this stage, complex polymers such as cellulose, hemicellulose, and lignin decompose into smaller molecular compounds through a series of reactions including depolymerization, fragmentation, and secondary cracking. The choice of reactor design such as fixed-bed, fluidized-bed, rotary-kiln, or auger-type plays a crucial role in determining the heat transfer efficiency, residence time, and product distribution (Raza et al., 2021). For example, fluidized-bed reactors offer excellent temperature uniformity and fast heat transfer, making them suitable for fast pyrolysis aimed at maximizing liquid yields (Zhou et al., 2022). Process parameters such as heating rate and residence time are particularly influential. Higher heating rates and shorter vapor residence times generally favor bio-oil production, while slower heating and longer residence tend to increase biochar yield (Chen et al., 2022).

Following pyrolysis, the resulting products are separated based on their phase. The pyrolysis vapors are condensed using heat exchangers or condensers to recover liquid bio-oil, while the remaining non-condensable gases are collected or flared. The design and configuration of the condensation system such as using counter-current or parallel flow can significantly affect the efficiency of vapor-to-liquid conversion. Further refinement of the bio-oil may be conducted via distillation to isolate specific chemical fractions based on their boiling points.

Reaction Kinetics of Biomass Pyrolysis

Biomass pyrolysis is a complex process reaction involving the thermal decomposition of organic materials in the absence of oxygen, leading to the production of biochar, bio-oil, and gases. There are several models developed to represent the pyrolysis reaction kinetics such as One-Step Global Kinetic Model, Distributed Activation Energy Model (DAEM), and Avrami-Erofeev Model (Fan et al., 2022; Fu et al., 2022). One-Step Global Kinetic Model is the most common used. this model is used to determine kinetic parameters such as pre-exponential factor, activation energy, and reaction order. It has been applied to various biomass samples, showing that activation energy varies significantly among different types of biomass. Activation energy values for biomass pyrolysis can vary widely. For example, empty fruit bunches have activation energies ranging from 10.2 to 64.6 kJ/mol, while coconut shells range from 18.7 to 186.2 kJ/mol (Supee & Zaini, 2023). The order of reaction for different biomass components can be assumed to be 1 for cellulose, hemicellulose, and lignin (Cano-Pleite et al., 2021). The multistep kinetic scheme of cellulose pyrolysis, with a lumped description of the released species, is reported in Table 2 (Ranzi et al., 2008). The rate parameters of the reactions are mainly derived from TG experiments at different heating rates, as well as obtained from a semidetailed kinetic scheme.

DWSIM Simulation

Process Flow Diagram

A PFD was developed using DWSIM, an open-source chemical process simulator, to model the pyrolysis of OPEFB as presented in Figure 1. The simulation was designed to evaluate the effect of operating temperature on the distribution of pyrolysis products. In the model, OPEFB with defined proximate, ultimate, and compositional data was fed into a pyrolysis reactor. The reactor simulates the thermochemical decomposition of

Table 2. Lumped kinetic scheme of cellulose, hemicellulose, and lignin pyrolysis.

reaction	rate
Cellulose → active-Cellulose	$k = 8 \times 10^{13}\exp(-46000/RT)$
Active-Cellulose → 0.95 CH_3COOH + 0.25 $C_2H_2O_2$ + 0.2 CH_3CHO + 0.2 C_3H_6O + 0.25 furfural + 0.2 CO_2 + 0.15 CO + 0.1 CH_4 + 0.9 H_2O + 0.65 Char	$k = 1 \times 10^{9}\exp(-30000/RT)$
Cellulose → 5 H_2O + 6 Char	$k = 8 \times 10^{7}\exp(-32000/RT)$
Hemicellulose → 0.1 HemCell1 + 0.6 HemCell2	$k = 1 \times 10^{10}\exp(-31000/RT)$
HemCell1 → 2.5 H_2 + 0.125 H_2O + CO + CO_2 + 0.5 CH_2O + 0.25 CH_3OH + 0.125 C_2H_5OH + 2 Char	$k = 3 \times 10^{9}\exp(-27000/RT)$
HemCell2 → 1.5 H_2 + 0.125 H_2O + 0.2 CO_2 + 0.7 CH_2O + 0.25 CH_3OH + 0.125 C_2H_5OH + 0.8 CO_2 + 0.8 COH2 + 2 Char	$k = 1 \times 10^{10}\exp(-33000/RT)$
Lignin → 0.7 H_2 + H_2O + 0.2 CH_2O + 0.5CO+ 0.2 CH_2O+ 0.4CH_3OH + 0.2 CH_3CHO + 0.2 $C_3H_6O_2$ +.4 CH_4 + 0.5 C_2H_4 + CO + 0.5 COH_2 + 6 Char	$k = 1.2 \times 10^{9}\exp(-30000/RT)$

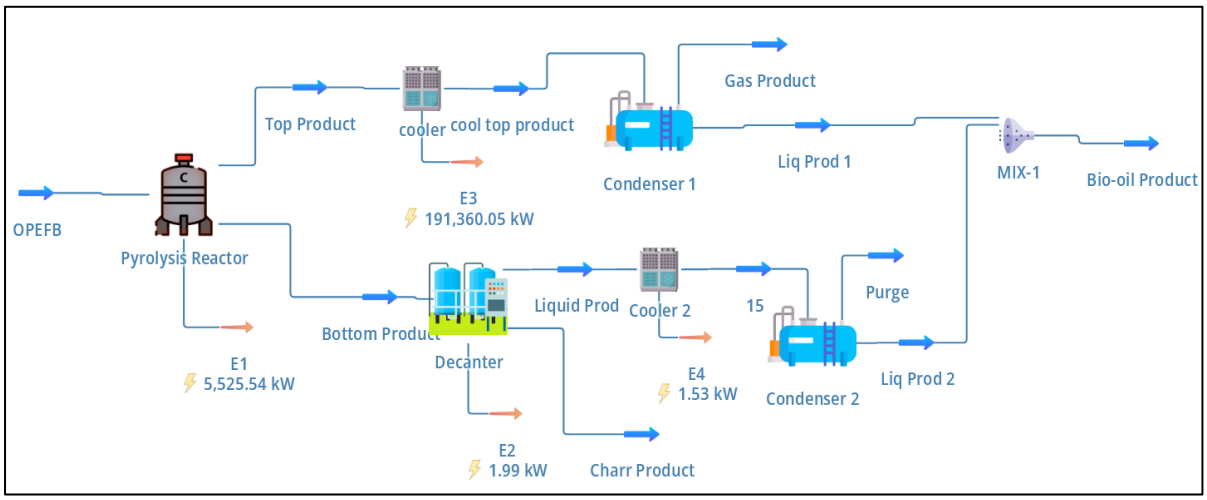

Figure 1. Process flow diagram of pyrolysis process in DWSIM software

biomass in an oxygen-free environment at varying temperatures. The reactor produces two main output streams: A top product stream, primarily consisting of pyrolysis vapors and gases. A bottom product stream, comprising heavier liquid fractions and solid biochar.

The top product stream exits the reactor at high temperature and is routed through a cooling unit, where it is cooled to approximately 30 °C to simulate condensation of volatile components. The heat removed from this stream is considered recoverable and may be reused for utility purposes such as in a waste heat boiler or feedstock drying system. Following cooling, the resulting two-phase mixture (gas and condensed vapor) is separated using a gas-liquid separator. This unit separates the stream into a non-condensable gas product and a light liquid fraction, representing part of the bio-oil. The bottom product from the reactor, containing a mixture of bio-oil and biochar, is processed in a decanter unit. This unit performs a phase separation based on density differences to isolate the heavy bio-oil fraction from the solid biochar product.

Selection of Components and Property Packages

In the simulation, the main biomass constituents were modelled using their representative monomeric forms: cellulose was represented as glucose, and hemicellulose as xylose. For lignin, a hypothetical component was created using DWSIM compound creator, based on available physicochemical property data to approximate the behaviour of kraft lignin. The major pyrolysis products included in the model such as water, hydrogen, carbon dioxide (CO_2), carbon monoxide (CO), furfural, methanol, formaldehyde, acetaldehyde, propionaldehyde, ethylene, and ethylene glycol were selected from the

existing DWSIM component database. For glyoxal ($C_2H_2O_2$), which is not available by default in DWSIM, the component was imported using data obtained from reliable online chemical property databases, specifically KDB (https://www.mdlkdb.com/) and Cheméo (https://www.chemeo.com/). The Peng–Robinson equation of state (EOS) was selected as the property package for this simulation (Andreasen, 2022b). This EOS is well-suited for modelling gas–liquid equilibria and handling systems involving light gases, condensable vapours, and complex hydrocarbon mixtures, making it appropriate for the multiphase nature of biomass pyrolysis products.

Assumptions and Simplifications Made in The Simulation

To ensure effective simulation within the capabilities of DWSIM, several assumptions and simplifications were applied. The pyrolysis process was modelled as a non-catalytic, single-step reaction, representing the overall thermal degradation of biomass components into simplified product groups. The pyrolysis reactor was treated as a stoichiometric conversion reactor, with product yield distributions assigned based on values reported in relevant literature.

In this approach, the reaction kinetics were simplified to a first-order reaction model for all biomass constituents, where the conversion was treated as a function of temperature. Accordingly, the general rate expression is described by Eq. (1).

$$-\frac{dC_A}{dt} = k(T)C_A \qquad (1)$$

In steady-state continuous operation, the rate equation can be expressed in terms of conversion (X) as presented in Eq. (2) where τ is the residence time in the reactor. In this simulation, the pyrolysis process was modeled as fast pyrolysis, with a vapor residence time of 1 second in the reactor retort. This value was selected based on typical fast pyrolysis conditions reported in the literature, which range from 0.5 to 3 seconds (Marathe et al., 2020).

$$\ln(1-X) = -k(T)\tau \qquad (2)$$

By incorporating the Arrhenius equation for temperature-dependent rate constants ($k(T)$), the expression becomes Eq. (3).

$$X(T) = 1 - \exp\left[\left(A_0 \exp\left(\frac{-E}{RT}\right)\right)\tau\right] \qquad (3)$$

To further simplify the model, heat losses to the surroundings were neglected, and the reactor was assumed to operate under isothermal conditions with a pre-heated biomass feed. Heat flow across the unit was calculated based on the outlet stream temperature for designated cooling units. Separation units (gas-liquid separator and decanter) were assumed to operate under ideal phase separation conditions, with no mechanical or thermal inefficiencies considered. This allowed the simulation to focus on mass and energy balances without introducing complexity associated with separation dynamics.

RESULTS AND DISCUSSION

Base Case Simulation Results

The base case simulation of OPEFB pyrolysis was conducted at an operating temperature of 400 °C (673.15 K), with a biomass feed rate of 100 kg/s. The overall material balance for the process is summarized in Table 3. Following thermal decomposition, the reactor produced a top product stream (71.26% by mass) consisting predominantly of pyrolysis vapors and gases, and a bottom product stream (28.74% by mass) comprising heavy liquid and solid char. The top product stream was rich in volatile organic compounds (VOCs), non-condensable gases, and water vapor, while the bottom product primarily consisted of char and residual unconverted cellulose. From the simulation, the conversion of cellulose was approximately 96%, while hemicellulose and lignin were almost completely decomposed, with conversions approaching 100%. This is consistent with the higher thermal reactivity of hemicellulose and lignin compared to cellulose under pyrolysis conditions.

Subsequent separation stages—including cooling, gas-liquid separation, and decantation—resulted in the final distribution of products was Gas product up to 52.77%, Bio-oil product up to 18.53%, and Bio-char product up to 28.71%. The gas product was primarily composed of hydrogen (H_2, 24.4 mol%) and carbon monoxide (CO, 15.66 mol%), followed by carbon dioxide (CO_2, 10.3 mol%), methane (CH_4, 8.5 mol%), and trace amounts of light organics such as methanol,

Table 3. Material balance of the simulation process using base case.

Stream Number	1	2	3	4	5	6	7	8	9	10
Stream Name	**OPEFB**	**Top Product**	**Bottom Product**	**cool top product**	**Liquid Prod**	**Gas Prod**	**Liq Prod 1**	**Char Product**	**Liq Prod 2**	**Bio-Oil Prod**
Temperature, K	673.15	673.15	673.15	323.15	673.15	323.15	323.15	673.15	303.15	323.111
Pressure, Pa	101325	101325	101325	101325	101325	101325	101325	101325	101325	101325
Mass Flow, kg/s	100	71.26	28.74	71.26	0.03	52.77	18.50	28.71	0.03	18.53
Molar Flow, mol/s	520.55	3075.42	1094.25	3075.42	1.09	2442.43	632.99	1093.15	1.09	634.08
Volumetric Flow, m^3/s	0.12	169.87	0.02	64.78	0.06	64.76	0.02	0.02	0.00	0.02
Molar fraction:										
Cellulose	0.4907	0.0001	0.0847	0.0001	0.0000	0.0000	0.0004	0.0848	0.0000	0.0004
Glyoxal	0.0000	0.0084	0.0000	0.0084	0.0000	0.0092	0.0055	0.0000	0.0000	0.0055
Hemicellulose	0.3846	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Lignin	0.1247	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Acetic acid	0.0000	0.0320	0.0000	0.0320	0.0002	0.0107	0.1142	0.0000	0.0002	0.1140
Acetaldehyde	0.0000	0.0157	0.0000	0.0157	0.0001	0.0186	0.0041	0.0000	0.0001	0.0041
Propanal	0.0000	0.0067	0.0000	0.0067	0.0004	0.0079	0.0021	0.0000	0.0004	0.0021
Furfural	0.0000	0.0084	0.0000	0.0084	0.0000	0.0025	0.0314	0.0000	0.0000	0.0313
Carbon dioxide	0.0000	0.0818	0.0000	0.0818	0.0006	0.1030	0.0000	0.0000	0.0002	0.0000
Carbon monoxide	0.0000	0.1244	0.0000	0.1244	0.0002	0.1566	0.0000	0.0000	0.0000	0.0000
Methane	0.0000	0.0683	0.0000	0.0683	0.0001	0.0859	0.0000	0.0000	0.0000	0.0000
Water	0.0000	0.2255	0.0008	0.2255	0.7783	0.0976	0.7189	0.0000	0.7798	0.7190
Char	0.0000	0.0000	0.9143	0.0000	0.0000	0.0000	0.0000	0.9152	0.0000	0.0000
Hydrogen	0.0000	0.2440	0.0000	0.2440	0.0013	0.3073	0.0000	0.0000	0.0000	0.0000
Formaldehyde	0.0000	0.1173	0.0000	0.1173	0.0002	0.1441	0.0138	0.0000	0.0002	0.0138
Methanol	0.0000	0.0323	0.0000	0.0323	0.0034	0.0300	0.0412	0.0000	0.0034	0.0411
Ethanol	0.0000	0.0125	0.0000	0.0125	0.0003	0.0112	0.0176	0.0000	0.0003	0.0176
Ethylene glycol	0.0000	0.0105	0.0002	0.0105	0.2150	0.0000	0.0507	0.0000	0.2154	0.0510
Ethylene	0.0000	0.0122	0.0000	0.0122	0.0000	0.0153	0.0000	0.0000	0.0000	0.0000

formaldehyde, glyoxal, ethylene, and acetaldehyde. These results align with experimental findings from previous studies that report H_2 and CO as the dominant gas species in pyrolysis of lignocellulosic biomass.

The bio-oil product, recovered from both the light liquid and heavy bottom liquid fractions, consisted of water (~71.9 mol%), followed by significant fractions of acetic acid, furfural, methanol, formaldehyde, and ethylene glycol. These compounds are known intermediates in fuel refining and chemical synthesis, highlighting the potential of pyrolysis oil as a feedstock for renewable platform chemicals, provided proper upgrading and purification steps are applied. The bio-char contained a high carbon content (91.5 mol%) with the remaining fraction attributed to residual cellulose (~8.48 mol%) and inorganic ash. This carbon-rich material has potential applications as a soil amendment, adsorbent, or solid biofuel, depending on its surface properties and ash content.

For comparison, catalytic pyrolysis has been shown to significantly alter product distribution. For instance, Hamdan et al. (2021) reported that catalytic pyrolysis of OPEFB using zeolite A at 400 °C yielded 42.7% bio-oil, 35.4% char, and 21.9% gas, demonstrating the influence of catalyst on reaction pathways and product selectivity. Overall, the simulation results provide valuable insights into the thermal conversion behavior of OPEFB under non-catalytic conditions and highlight the capability of open-source process simulation (DWSIM) to estimate product yields and compositions for process design and optimization.

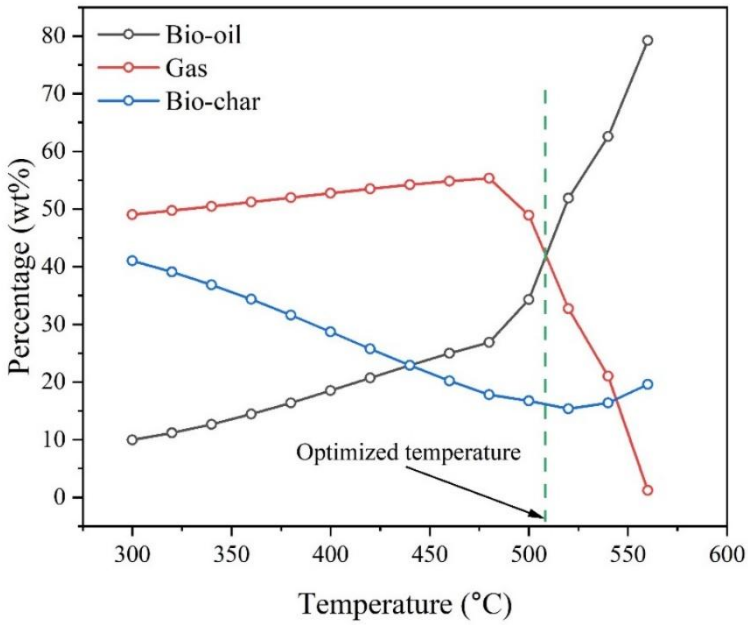

Figure 2. OPEFB pyrolysis products distribution at various operating temperatures.

Effect of Temperature on Product Distribution

Figure 2 illustrates the effect of pyrolysis temperature on the distribution of major products—bio-oil, gas, and bio-char—as a function of temperature ranging from 300 °C to 580 °C. The results demonstrate a clear temperature-dependent shift in product yields, indicating the influence of thermal severity on biomass decomposition pathways. At lower temperatures (< 400 °C), the process favors the formation of bio-char, which is consistent with the limited thermal degradation of biomass and the retention of solid carbonaceous residues. As temperature increases, bio-char yield steadily declines, indicating enhanced devolatilization and thermal cracking of the solid matrix. This trend is well-supported by prior studies; for instance, Raju et al. (2021) observed a sharp reduction in char yield above 500 °C due to intensified cracking and fragmentation of lignocellulosic structures.

The gas yield initially increases with temperature up to approximately 460 °C, likely due to the thermal decomposition of volatile organic matter, hemicellulose, and light oxygenated compounds. This is in agreement with the progressive breakdown of light organics and the formation of gases such as CO, CO_2, CH_4, and H_2. However, beyond 460 °C, gas yield begins to decline, which may be attributed to the secondary cracking of volatiles into liquid-phase bio-oil components or re-polymerization reactions. Such behavior suggests that condensable compounds become more dominant at elevated temperatures, especially around the optimized zone. The bio-oil yield shows a sharp increase between 450 °C and 520 °C, with a maximum near 510 °C, which represents the optimized pyrolysis temperature for producing a balanced output of bio-oil and gas, while minimizing bio-char. At this point, the conversion of biomass components into liquid intermediates is maximized, without excessive thermal degradation that could lead to further cracking into non-condensable gases. This observation is consistent with experimental studies on OPEFB pyrolysis. Sutrisno and Hidayat (2018) reported a maximum bio-oil yield of 44.5 wt% at 450 °C, while Sukiran et al. (2009) observed the highest yield of 42.28 wt% at 500 °C. These findings are in line with the simulated optimum shown in the current work. On the other hand, Kusworo et al. (2020) reported high gas yields up to 67.18 wt% at 600 °C, confirming the trend that extreme pyrolysis temperatures tend to favor gas production at the expense of liquid and solid yields. Overall, the figure demonstrates that 510 °C is an optimal condition for producing both bio-oil and gas in significant proportions while keeping bio-char yield minimal. This balanced product distribution is favorable for integrated biorefinery applications

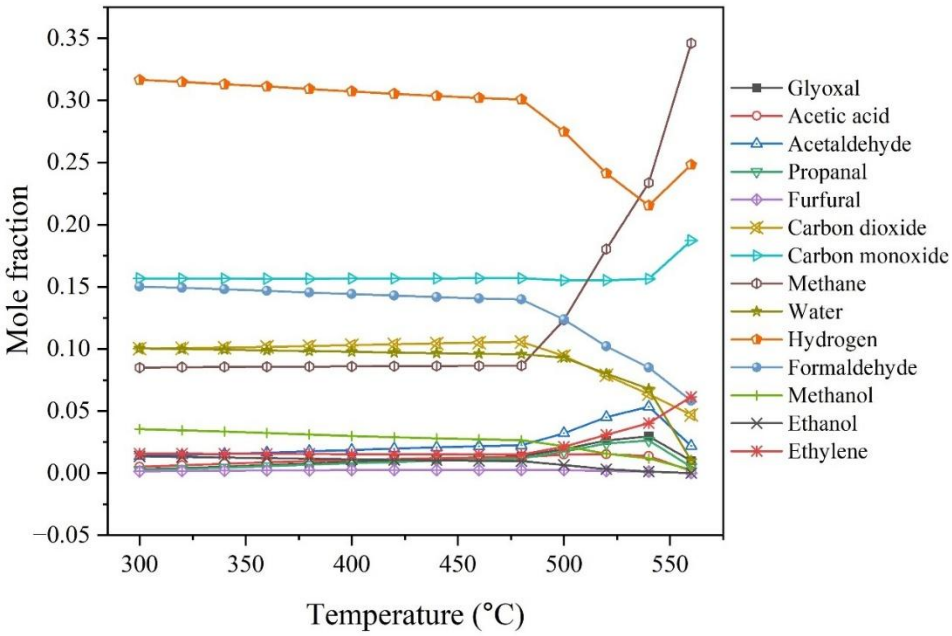

Figure 3. Gas yield composition at various pyrolysis temperature.

where both energy and chemical recovery are desired.

Effect of Temperature on Gas Products

The composition of pyrolysis gas products derived from oil palm empty fruit bunches (OPEFB) is significantly influenced by pyrolysis temperature, as illustrated in Figure 3. The figure shows the mole fractions of various gas-phase components as a function of temperature, ranging from 300 °C to 550 °C. Among the primary constituents, hydrogen (H_2) exhibits the highest mole fraction throughout the temperature range, remaining relatively stable at ~0.31 until 480 °C, after which it drops sharply. A similar trend is observed for carbon dioxide (CO_2), whose mole fraction also declines noticeably beyond 480 °C. This decrease in both H_2 and CO_2 above 480 °C is likely due to the enhanced formation of methane (CH_4) via the methanation reaction in Eq. (4).

$$CO_2 + 2\ H_2 \rightarrow CH_4 + O_2 \qquad (4)$$

This is supported by the corresponding increase in CH_4 mole fraction, which peaks at higher pyrolysis temperatures. The data suggest a temperature-driven shift in reaction pathways that promotes hydrocarbon gas formation over molecular hydrogen and carbon oxides at elevated temperatures.

Carbon monoxide (CO), another major gaseous product, shows a steady increase across the temperature range, indicating enhanced devolatilization and secondary cracking reactions at higher temperatures. In contrast, water vapor (H_2O) remains nearly constant (~0.10 mole fraction), which may indicate a balance between moisture release and secondary steam-reforming reactions at the tested temperatures. Other detected species such as acetic acid, acetaldehyde, methanol, ethanol, formaldehyde, and furfural appear in lower mole fractions but contribute significantly to the overall chemical diversity of the pyrolysis vapors. These oxygenated compounds originate primarily from the decomposition of hemicellulose and cellulose. Notably, glyoxal mole fraction increases substantially beyond 500 °C, indicating its formation as a secondary product from the degradation of more complex volatile intermediates. Ethylene (C_2H_4) and methanol also exhibit an upward trend at higher temperatures, albeit in relatively low concentrations, consistent with the thermal cracking of heavy volatile organics. The emergence of light hydrocarbons at elevated temperatures aligns with findings from Zailani et al. (2017) and Sukiran et al. (2014), who observed higher yields of CH_4, C_2H_6, and C_2H_4 at temperatures exceeding 500 °C.

According to Handoko et al. (2021), the typical syngas composition from OPEFB pyrolysis includes CH_4 (13–17% vol), H_2 (28–33% vol), CO (17–26% vol), and CO_2 (16–31% vol). The simulation results in this study closely reflect these experimental ranges, validating the model accuracy

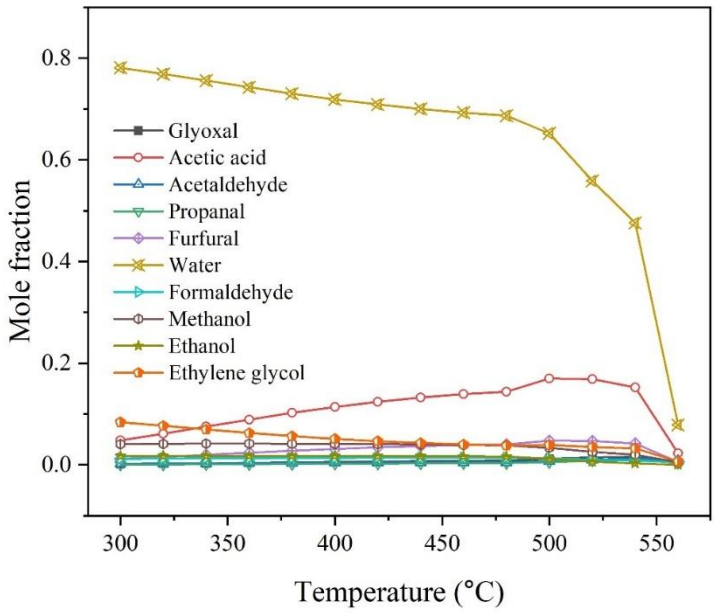

Figure 4. Bio-oil yield composition at various pyrolysis temperature.

and emphasizing the potential of OPEFB as a viable feedstock for syngas production. In summary, pyrolysis temperature not only affects the overall gas yield but also governs the distribution and conversion pathways of individual gaseous species. Operating at temperatures between 500 °C and 520 °C offers a favorable balance between light hydrocarbon gas generation and syngas quality, which is critical for downstream applications in combustion, reforming, or synthesis processes.

Effect of Temperature on Bio-oil Products

Bio-oil derived from the pyrolysis of Oil Palm Empty Fruit Bunches (OPEFB) is a complex mixture of oxygenated compounds, including organic acids, aldehydes, ketones, alcohols, furans, and water. The composition of these components is strongly influenced by pyrolysis temperature, as shown in Figure 4, which illustrates the variation in mole fractions of selected bio-oil components over a temperature range of 300–550 °C. Water is the most dominant component in bio-oil across all temperatures, starting at approximately 0.75 mole fraction at 300 °C. However, its concentration decreases steadily with increasing temperature, reaching a sharp decline beyond 520 °C. This trend suggests that at elevated temperatures, water may either vaporize into the gas phase or participate in secondary cracking and reforming reactions that reduce its concentration in the liquid phase.

Among the oxygenated compounds, acetic acid shows a clear increasing trend up to around 500 °C, where it reaches its maximum mole fraction (~0.13), followed by a steep decline at temperatures above 520 °C. This behavior may indicate thermal degradation or transformation into lighter compounds or gases at higher temperatures. Acetic acid is a major product of hemicellulose degradation, and its high concentration reinforces the significant contribution of hemicellulosic structures in OPEFB to bio-oil formation. Furfural, a key platform chemical derived from lignocellulosic biomass, is observed at consistent levels (~0.01 mole fraction) across a broad temperature range. Furfural is primarily produced through the acid-catalyzed dehydration of pentoses like xylose from hemicellulose. It remains stable in the bio-oil at moderate pyrolysis temperatures but can degrade or volatilize at temperatures above 520 °C. The consistent presence of furfural and alcohol derivatives such as methanol, ethanol, and ethylene glycol confirmed the pyrolytic decomposition of both cellulose and hemicellulose, as also reported by Modak et al. (2023).

Methanol, formaldehyde, and ethylene glycol exhibit modest increases with temperature, which is typical of the thermal cracking of carbohydrate polymers. Their stable formation across the temperature range suggests limited secondary reactions, except for formaldehyde, which shows a slight increase above 480 °C. Aromatic and aliphatic compounds, such as phenol and benzene, which are not explicitly shown in this figure but reported in the literature, contribute significantly to the heating value and chemical reactivity of bio-oil. Faisal et al. (2020) noted that

phenol peaks at 340 °C, while acetic acid reaches its maximum at 320 °C. While these specific values differ slightly due to different experimental conditions and feedstock variability, the simulation results in this study are in agreement with the general temperature dependency trends for bio-oil composition. Moreover, Yanti et al. (2019) highlighted the presence of aliphatic and aromatic hydrocarbons in bio-oil, which were confirmed in this study through the identification of intermediate compounds like ethanol and furfural. These compounds not only enhance the energy content of bio-oil but also improve its potential as a renewable chemical feedstock. The results highlight the importance of temperature optimization during pyrolysis to control the quality and yield of bio-oil. Temperatures in the range of 450–510 °C are most favorable for achieving a balanced bio-oil composition with substantial yields of water, acids, and platform chemicals while minimizing degradation into gas-phase products.

Effect of Temperature on Bio-char product

The pyrolysis temperature plays a critical role in determining the composition and properties of biochar derived from Oil Palm Empty Fruit Bunches (OPEFB). As shown in Figure 5, the mole fractions of cellulose, hemicellulose, lignin, and carbon in the residual solid phase vary significantly with temperature, reflecting the thermal decomposition behavior of lignocellulosic components during pyrolysis. At temperatures below 500 °C, carbon content in the solid product steadily increases, reaching a maximum mole fraction close to 0.95. This increase is attributed to the progressive thermal decomposition of cellulose and hemicellulose, which volatilize more readily, leaving behind a carbon-enriched residue. However, beyond 520 °C, a sharp decline in carbon content is observed. This trend suggests that at elevated temperatures, carbon begins to react with evolved gases, particularly water vapor and hydrogen, through gasification reactions Eq. (5) – (6).

$$C + H_2O \rightarrow CO + H_2 \quad (5)$$

$$C + 2\,H_2 \rightarrow CH_4 \quad (6)$$

These reactions lead to the formation of syngas ($CO + H_2$) and methane, effectively reducing the fixed carbon content in the residual char and increasing the yield of gaseous products. This aligns with the concurrent increase in methane mole fraction seen in the gas phase product analysis at high temperatures. The cellulose fraction shows a continuous decrease from 300 to 500 °C, indicating extensive decomposition under thermal stress. However, a residual amount remains up to 520 °C, likely due to incomplete breakdown or re-condensation of volatile intermediates. A sharp increase in the cellulose fraction at temperatures above 540 °C may reflect simulation artifacts or reformation of heavier compounds under extreme thermal cracking conditions. Hemicellulose is nearly completely decomposed across all temperatures, consistent with its known thermal instability and lower decomposition temperature (~200–350 °C). This behavior supports the role of hemicellulose as a primary source of volatile compounds in bio-oil and gas production. Lignin, by contrast, exhibits greater thermal stability and decomposes over a broader temperature range. Its mole fraction remains relatively constant at lower temperatures, followed by a noticeable increase beyond 540 °C. This may reflect the accumulation of unconverted aromatic residues or simulation-based estimation of persistent solids.

These results are consistent with findings by Marhani et al. (2022) and Bakhtiar et al. (2019), who reported that while increasing pyrolysis temperature reduces biochar yield, it enhances its fixed carbon content, alkalinity, and surface area—attributes beneficial for applications such as soil amendment, carbon sequestration, and bioenergy generation. The operating temperature around 500–520 °C represents a critical threshold in OPEFB pyrolysis, beyond which substantial transformation of solid carbon into gaseous products occurs. Understanding these temperature-dependent changes in biochar composition is essential for tailoring pyrolysis conditions to target specific applications.

Potential of the future development

As the world largest producer of palm oil, Indonesia generates vast amounts of oil palm biomass, particularly OPEFB, which remain underutilized. Pyrolysis offers a sustainable route to convert this biomass into bio-oil, biochar, and syngas, supporting national goals in renewable energy and waste valorization. Future developments should focus on enhancing reactor design through improved kinetic and heat transfer

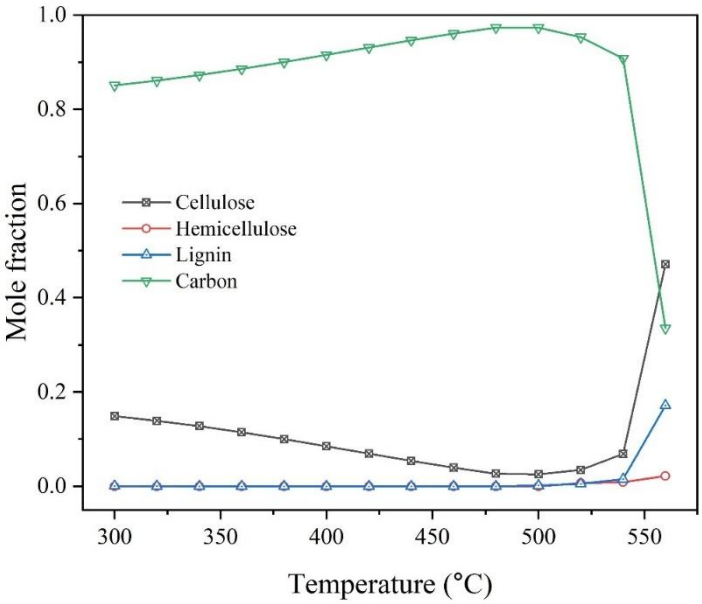

Figure 5. Bio-char components profile at various pyrolysis temperature.

models to optimize product yields. Integration of waste heat recovery and biomass pretreatment technologies, such as torrefaction, can significantly improve energy efficiency (Xing et al., 2021). The use of cost-effective catalysts, especially from local natural resources, in catalytic pyrolysis could improve bio-oil quality and broaden its applications (Fadillah et al., 2021). Upgrading methods such as hydrodeoxygenation and emulsification should also be explored to enhance bio-oil stability and usability as renewable fuel (Hansen et al., 2020). Biochar development should target high-value uses, including soil amendment, pollutant adsorption, and composite material reinforcement (Yasim-Anuar et al., 2022). Comprehensive techno-economic and life cycle assessments will be essential to guide commercial adoption. Finally, the integration of open-source simulation tools and digital optimization can facilitate scalable and cost-effective deployment, particularly for rural and industrial applications in Indonesia.

CONCLUSION

This study successfully simulated the pyrolysis of OPEFB using the open-source chemical process simulator DWSIM. The simulation model incorporated key biomass constituents—cellulose, hemicellulose, and lignin—represented by their monomeric forms and hypothetical compounds. The process flow included pyrolysis reaction, cooling, and gas-liquid-solid separation units. The simulation results demonstrated that at an optimal pyrolysis temperature of 510 °C, a balanced product distribution was achieved: 52.77 wt% gas, 18.53 wt% bio-oil, and 28.71 wt% biochar. Temperature had a significant influence on the decomposition behavior and product yield, with higher temperatures favoring gas production and reducing char yield. The use of DWSIM proved effective for modeling biomass pyrolysis, offering an accessible and cost-free alternative to commercial simulators. It enables researchers, especially in resource-limited settings, to perform process design, sensitivity analysis, and conceptual evaluations. However, the simulation involved simplifications and assumptions, including first-order reaction kinetics, ideal separation, isothermal operation, and the exclusion of catalytic effects. These limitations affect the predictive accuracy of product composition and thermodynamic behavior. For future work, the model should be refined with detailed kinetic mechanisms, non-ideal thermodynamics, and dynamic heat profiles. Experimental validation is crucial to confirm simulation accuracy. Moreover, integrating the pyrolysis process with downstream upgrading units (e.g., distillation, hydrogenation) and techno-economic assessments will enhance its relevance for industrial-scale deployment.

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