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Steam Explosion of Palm Oil Mesocarp Fiber: A Simulation Study

Nur Yasmin Najihah Yahaya
Asmida Ideris*
Faculty of Chemical and Process Engineering Technology,
Universiti Malaysia Pahang Al-Sultan Abdullah, Lebuh Persiaran Tun Khalil Yaakob
26300, Kuantan, Pahang, Malaysia
*e-mail: asmida@umpsa.edu.my

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Abstract. Palm oil mesocarp fiber (POMF), a lignocellulosic biomass generated in large quantities during palm oil production, is a potential feedstock for sugar production via steam explosion. In this study, the steam explosion of POMF was simulated using Aspen Plus® to evaluate the effects of POMF composition, steam explosion temperature (110–220°C), and residence time (3.5–20 min) on cellulose and hemicellulose conversions as well as on the yields of sugars and degradation products. Variations in POMF composition had no significant impact on cellulose or hemicellulose conversion, nor on the resulting product yields. Across all samples, glucose yields remained constant at approximately 14%, while xylose yields remained stable at approximately 6%. Furfural and 5-HMF yields were minimal at ~0.5% and ~0.2%, respectively. In contrast, product yields were highly sensitive to steam explosion temperature. Glucose yield increased moderately from ~12.7 to ~14.3% at intermediate temperatures before declining sharply between 170 and 210°C. Xylose increased from 0.47 to 10.1% as the temperature rose from 130 to 160°C, then decreased substantially at higher temperatures. At elevated temperatures, sugars became unstable and degraded, leading to significant increases in furfural and 5-HMF formation above 160°C. Residence time had a stronger influence than temperature. Prolonged exposure intensified sugar degradation, with glucose decreasing from ~14.1 to 2.3% and xylose decreasing to 1.4% as residence time increased from 3.5 to 20 min. Correspondingly, furfural and 5-HMF yields increased gradually with time, indicating enhanced secondary degradation pathways. Overall, the Aspen Plus® model successfully described the steam explosion behavior of POMF over a wide range of process conditions. While POMF composition exerted minimal influence, both steam explosion temperature and residence time strongly affected sugar release and the formation of degradation products.

Keywords: Aspen Plus, Degradation Products, Palm Oil Mesocarp Fiber, Steam Explosion, Sugars

INTRODUCTION

The palm oil industry in Malaysia generates substantial quantities of biomass waste, primarily consisting of empty fruit bunches, palm oil mesocarp fiber (POMF), palm kernel shells, and palm oil mill effluent (Parthasarathy *et al*., 2024). POMF is a lignocellulosic residue rich in cellulose, hemicellulose, and lignin. Despite its

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abundance, only about 10% of POMF is currently recovered for electricity generation, while the remaining 90% is discarded (Ahmad Rizal *et al*., 2018). The continuous accumulation of untreated POMF and the common practice of open incineration pose environmental concerns, particularly air pollution. Therefore, converting POMF into higher-value products is essential to improve waste management and enhance resource utilization within the palm oil sector.

Rich in cellulose and hemicellulose, POMF can be effectively converted into fermentable sugars via steam explosion. Steam explosion is an autohydrolysis-based process in which lignocellulosic biomass is exposed to high temperatures (110–260 °C) and high-pressure steam (7–50 atm) for short residence times (30 s–20 min). This process is considered environmentally friendly as it operates without the need for additional chemical reagents. During the process, the biomass is saturated with high-pressure steam and then subjected to rapid pressure release, which disrupts the lignocellulosic matrix. Sudden decompression enhances the breakdown of cellulose and hemicellulose, promoting the release of monomeric sugars without the need for external catalysts (Keskin *et al*., 2019). As a result, steam explosion depolymerizes polysaccharides into fermentable sugars such as glucose and xylose, which can be further utilized as substrates for bioproduct fermentation (Ahmad Rizal *et al*., 2018).

Nevertheless, steam explosion is technically challenging to operate, as it relies on high-pressure, high-temperature steam, which demands robust, expensive equipment and stringent safety systems. This has made it difficult to vary the process conditions for optimization purposes. Therefore, Aspen Plus® simulation is a promising option for studying steam explosion due to its flexibility, reliability, safety, and ease of scale-up. Additionally, the composition of POMF varies according to environmental and cultivation factors, leading to fluctuations in its cellulose, hemicellulose, and lignin content *(Asyraf et al*., 2023). These compositional variations make it challenging to determine the optimum steam explosion conditions accurately. Simulation using Aspen Plus® provides an effective approach for predicting these optimal parameters. By integrating experimental compositional data with thermodynamic and kinetic models, Aspen Plus® systematically evaluates the effects of operating parameters and their interactions that are difficult to observe experimentally and predicts product distributions with high accuracy. Consequently, Aspen Plus® facilitates more efficient, cost-effective optimization of steam explosion conditions, reducing the need for extensive trial-and-error experiments while improving reliability in process design and scale-up.

The steam explosion process consists of several key stages: (1) the penetration of sub-critical water into the lignocellulosic structure, (2) the autohydrolysis of cellulose, hemicellulose, and associated linkages, and (3) a rapid depressurization step that induces mechanical rupture of the biomass matrix. Very often, empirical optimization of steam explosion parameters relies on hydrolysis kinetics, which are strongly dependent on both residence time and temperature. The commonly used severity factor is derived from an Arrhenius-type kinetics assuming a single overall reaction with a constant activation energy (Ziegler-Devin *et al*., 2021). In practice, the simultaneous hydrolysis of cellulose and hemicellulose must be considered, as well as the subsequent degradation of released sugars into inhibitory

by-products such as furfural ($C_5H_4O_2$), acetic acid ($C_2H_4O_2$), and 5-hydroxymethylfurfural (5-HMF, $C_6H_6O_3$). Accounting for these parallel and consecutive reactions is crucial for accurately evaluating steam explosion severity and predicting product yields.

In Aspen Plus® simulation, cellulose and hemicellulose are represented by glucan ($C_6H_{10}O_5$) and xylan ($C_5H_8O_4$), respectively. Meanwhile, lignin is expressed as a phenylpropane monomer (Adeniyi and Ighalo, 2020; Kuo and Yu, 2020; Li *et al*., 2019). The possible reactions involved in the steam explosion, along with the kinetics data of glucan and xylan hydrolysis and the degradation reactions, are provided by equations Eq. (1)-(8) (dos Santos Rocha *et al*., 2017). In this study, the first-order reaction rate and the Arrhenius equation were used to model the steam explosion of biomass.

Glucan ($C_6H_{10}O_5$) is hydrolyzed to glucose molecules ($C_6H_{12}O_6$) while xylan ($C_5H_8O_4$) is hydrolyzed into xylose ($C_5H_{10}O_5$) (Eq. (1) and Eq. (2)). 5-HMF ($C_6H_6O_3$) is the degradation product of glucose and furfural ($C_5H_4O_2$) is produced from the degradation of xylose (Eq. (3) and Eq. (4)). Meanwhile, while acetic acid ($C_2H_4O_2$) si produced through the degradations of xylose and glucose (Eq. (5) and Eq. (6)) and the hydrolysis of furfural and 5-HMF (Eq. (7) and Eq. (8)).

Hydrolysis of glucan to glucose:

$$C_6H_{10}O_5 + H_20 \rightarrow C_6H_{12}O_6 \quad (1)$$

k=0.055 min^{-1} (180°C)
Ea=105.6 kJ/mol

Hydrolysis of xylan to xylose:

$$C_5H_8O_4 + H_20 \rightarrow C_5H_{10}O_5 \quad (2)$$

k=0.0073 min^{-1} (180°C)
Ea=220.23 kJ/mol

Degradation of glucose to 5-HMF:

$$C_6H_{12}O_6 \rightarrow C_6H_6O_3 + 3H_20 \quad (3)$$

k=0.0023 min^{-1} (180°C)
Ea = 181.35 kJ/mol

Degradation of xylose to furfural:

$$C_5H_{10}O_5 \rightarrow C_5H_4O_2 + 3H_20 \quad (4)$$

k=0.0097 min^{-1} (180°C)
Ea = 122.57 kJ/mol

Degradation of xylose to acetic acid:

$$C_5H_{10}O_5 \rightarrow 2C_2H_4O_2 + CO + H_2 \quad (5)$$

k=0.0139 min^{-1} (180°C)
Ea = 146.47 kJ/mol

Degradation of glucose to acetic acid:

$$C_6H_{12}O_6 \rightarrow 2C_2H_4O_2 + 2CO + 2H_2 \quad (6)$$

k=0.0531 min^{-1} (180°C)
Ea = 118.98 kJ/mol

Hydrolysis of furfural to acetic acid:

$$C_5H_4O_2 + 3H_20 \rightarrow 2C_2H_4O_2 + CO + H_2 \quad (7)$$

k=0.0371 min^{-1} (180°C)
Ea = 119.91 kJ/mol

Hydrolysis of 5-HMF to acetic acid:

$$C_6H_6O_3 + 2H_20 \rightarrow 2C_2H_4O_2 + 2CO + 2H_2 \quad (8)$$

k=0.0531 min^{-1} (180°C)
Ea = 266.17 kJ/mol

The objective of this study is to evaluate the steam explosion behavior of palm oil mesocarp fiber (POMF) under varying biomass compositions, steam explosion temperatures, and residence times. Aspen Plus® process simulation software was employed to predict the influence of these parameters on hemicellulose and cellulose conversions, as well as on the formation of monomeric sugars and secondary degradation products.

MATERIALS AND METHODS

Material Composition

The POMFs used in this study were sourced from palm oil mills at Serting Hilir, FELDA Serting, and Sime Darby Selangor. Both palm oil mills at FELDA Serting, Serting Hilir, were located in Negeri Sembilan, Malaysia, while Sime Darby Selangor was located in Selangor, Malaysia. The compositions of POMF were derived from various sources and are listed in Table 1.

Table 1. POMF compositions from various sources

Sources	Cellulose (%)	Hemi-cellulose (%)	Lignin (%)	References
Serting Hilir	25.0	25.7	49.3	(Rafein *et al.*, 2014)
FELDA Serting	42.8	33.1	24.1	(Iberahim *et al.*, 2013)
Sime Darby Selangor	28.8	25.3	45.9	(Nordin *et al.*, 2013)

Aspen Plus® Simulation

Aspen Plus® V12 simulation software (Aspen Technology Inc, US) was used to model the steam explosion of POMF. The simulator rigorously represented the process, performing thermodynamic calculations based on the physical properties of defined components. The thermodynamic property package selected for the simulations was the non-random two-liquid (NRTL) method, because the system consists of a liquid phase in equilibrium with steam as vapor and polar aqueous mixtures of water and sugars. Both RStoic and RBatch were used for the reactor models. Table 2 lists the model descriptions and operating conditions used in the simulation.

Figure 1 shows the Aspen Plus® process flowsheet for the POMF steam explosion. POMF feed into the RStoic (R-101) reactor model was set at 3722 tonne/year (Jafri *et al.*, 2021). The RStoic (R-101) operated at 100°C and 1 atm to remove the moisture from the POMF. The separator Sep (V-101) removed the moisture content based on the split fraction set. The second RStoic reactor model (R-102) operated at 25°C and 1 atm to convert the non-conventional compound of POMF (cellulose, hemicellulose and lignin) into its conventional compounds i.e. glucan, xylan and lignin. The POMF compositions of various sources were varied based on Table 1. Steam was supplied into the RBatch reactor model (R-103) at 110 to 210°C. Then, the abrupt pressure change was applied in the RBatch (R-103) from 22 to 1 atm. Sensitivity analysis was performed to vary the steam explosion temperature from 110 to 210ºC and residence time from 3.5 to 20 min at R-103.

Table 2. Aspen Plus model descriptions and operating conditions

Aspen Plus ID	Description	Operating conditions
RStoic (R-101)	To remove moisture in the POMF	T = 100ºC P = 1 atm
RStoic (R-102)	To decompose non-conventional compound (POMF) into its conventional compound (glucan, xylan, lignin)	T = 25ºC P = 1 atm
Sep (V-101)	To remove moisture from POMF	Split fraction H_2O = 1
Pump (P-101)	To increase the pressure to 22 atm	P = 22 atm
RBatch (R-103)	To perform the steam explosion process	T = 110 – 210ºC P = 22 to 1 atm t = 3.5 – 20 min

RBatch reactor model (R-103) enables kinetic-based modeling of batch hydrothermal reactions. In this configuration,

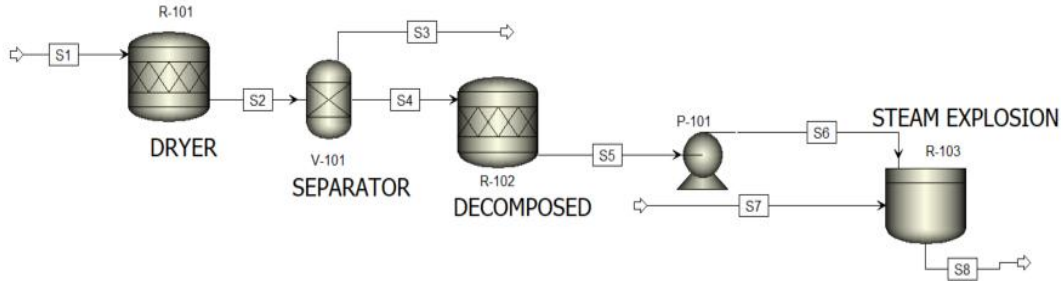


Fig. 1: Aspen Plus® process flowsheet for steam explosion of POMF

the depolymerization of cellulose and hemicellulose, the hydrolysis of glucan and xylan, and the formation of degradation products were represented by their corresponding kinetic constants and stoichiometries.

The molar flow rates (kmol/h) of the outlet stream from the batch reactor (RBatch) were obtained at Stream 8 (S8). Glucose, xylose, acetic acid, furfural, and 5-hydroxymethylfurfural (5-HMF) were quantified along with the conversions of cellulose and hemicellulose. Product yields (*Y*i) and reactant conversions (*X*i) were calculated using Eqs. (9)-(15).

$$Y_{Glucose}(\%) = \frac{F_{Glucose}}{F_{Glucan}} \times 100\% \quad (9)$$

$$Y_{Xylose}(\%) = \frac{F_{Xylose}}{F_{Xylan}} \times 100\% \quad (10)$$

$$Y_{A.Acid}(\%) = \frac{F_{A.Acid}}{2.5\,F_{Xylan}} \times 100\% \quad (11)$$

$$Y_{Furfural}(\%) = \frac{F_{Furfural}}{F_{Xylan}} \times 100\% \quad (12)$$

$$Y_{5-HMF}(\%) = \frac{F_{5-HMF}}{F_{Glucan}} \times 100\% \quad (13)$$

$$X_{cellulose} = \frac{F_{Glucan,in} - F_{Glucan,out}}{F_{Glucan,in}} \quad (14)$$

$$X_{hemicellulose} = \frac{F_{Xylan,in} - F_{Xylan,out}}{F_{Xylan,in}} \quad (15)$$

where *F*i are the molar amounts (kmol/h) of the substances.

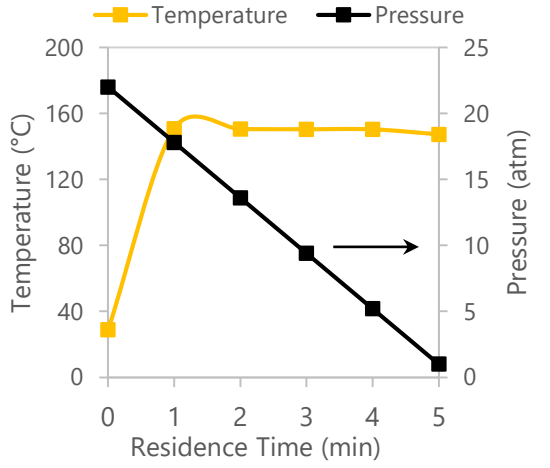
RESULTS AND DISCUSSIONS

Reactor (RBatch) Profiles

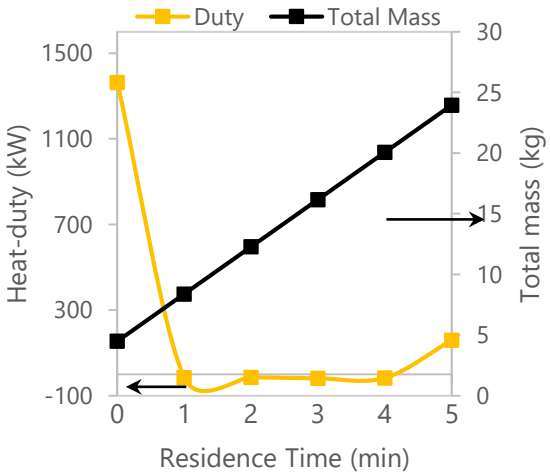
Aspen Plus® was used to obtain the operating-condition profiles for the steam explosion process. Figure 2(a) presents the temperature, pressure, heat duty, and total mass profiles for a batch reactor (RBatch) operated at 150 °C within a 5-min residence time. The reactor pressure decreased sharply from 22 to 1 atm during operation, reflecting the rapid depressurization characteristic of a steam explosion. The reactor temperature rose to 150°C within the first minute and remained stable until depressurization, during which it dropped to about 130°C. Figure 2(b) shows the corresponding heat duty and total mass profiles. An initial heat input of approximately 1400 kW was required to reach operating conditions, after which the system released heat at roughly 13 kW, followed by a smaller heat input of about 160 kW near the end of the cycle. The reactor's total mass increased gradually due to semi-batch feeding, and the accumulated products were discharged at the end of the residence period.

Figure 3 presents the steam consumption and average heat duty of the batch reactor (RBatch) across the evaluated temperature range. Steam usage remained nearly constant between 110 and 160°C at approximately 118 kg/h, but decreased slightly to around 110 kg/h as the operating

temperature increased from 160 to 210°C. This trend is attributed to the increase in the specific enthalpy of saturated steam at elevated temperatures. Consequently, a smaller steam mass is required to supply the necessary heat input. The higher specific enthalpy at elevated temperatures also accounts for the increase in average heat duty per cycle, as the reactor must meet a greater overall energy demand while relying on proportionally less steam mass (Zhong *et al.*, 2025).



(a)



(b)

Fig. 2: (a) Temperature and pressure profiles (b) Heat-duty and total mass profiles during semi-batch process of RBatch reactor at 150°C for 5 min residence time

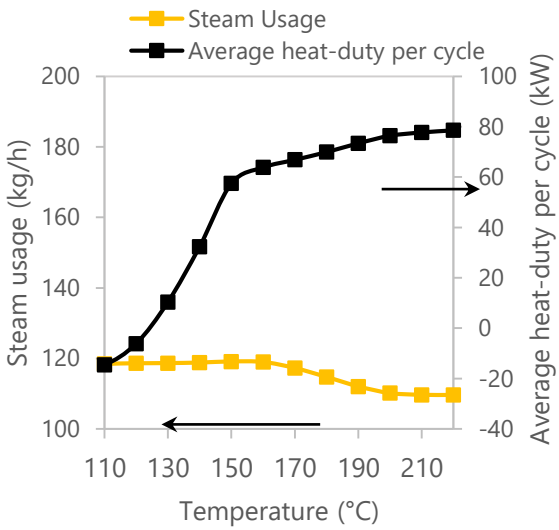


Fig. 3: Steam usage and average heat-duty per cycle for RBatch reactor at various temperatures (residence time: 3.5 min)

Data Validation

Model validation was conducted using hydrothermal pretreatment data from dos Santos Rocha *et al.* (2017) for sugarcane straw at 180, 195, and 210°C. From Figure 4, the simulated mass compositions of glucose, xylose, furfural, and 5-HMF showed good agreement with experimental trends, with increasing xylose, furfural, and 5-HMF and decreasing glucose at higher temperatures. However, the model failed to reproduce acetic acid formation, yielding zero values across all temperatures. This discrepancy stems from the kinetic scheme employed by dos Santos Rocha *et al.* (2017), which assumes that acetic acid originates from xylose degradation. In reality, acetic acid is primarily produced through hydronium-ion–catalyzed deacetylation of hemicellulose, specifically acetylated xylan chains (Sarker *et al.*, 2021). Overall, the simulation model can be considered adequate in predicting both sugars and degradation products generated from the steam explosion of POMFs.

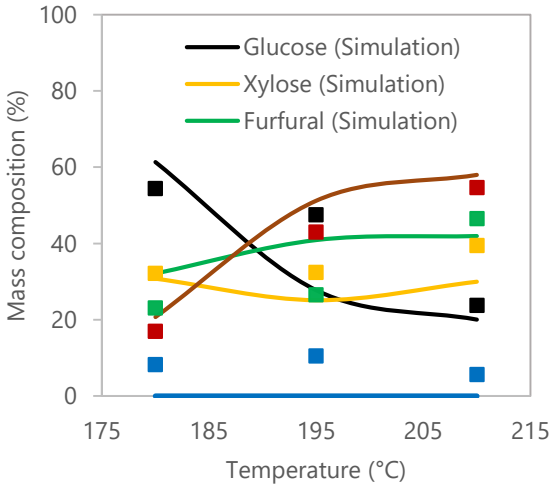


Fig. 4: Data validation

Effect of POMF Composition

Based on Table 1, the POMF samples from Serting Hilir and Sime Darby Selangor exhibited comparable compositions, whereas the POMF from FELDA Serting contained noticeably higher cellulose and hemicellulose contents. Figure 5 presents the simulated cellulose and hemicellulose conversions for the different POMF compositions.

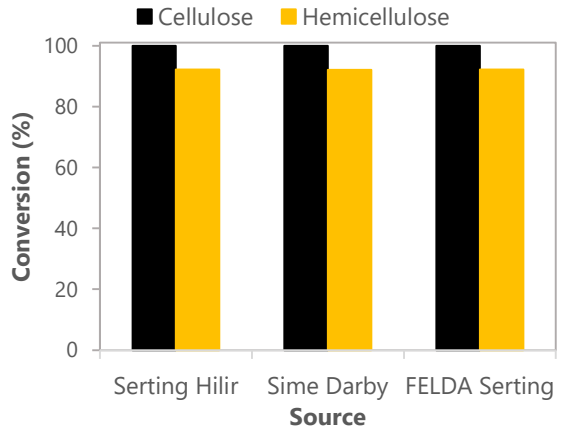


Fig. 5: Effect of POMF composition on hemicellulose and cellulose conversions (T=150˚C, t= 3.5 min)

Across all samples, cellulose conversion was slightly higher than hemicellulose conversion, with average values of approximately 100% and 92%, respectively. Although hemicellulose is typically more amorphous and possesses a lower degree of polymerization than cellulose (Zhao *et al.*, 2023), the results suggest the presence of an optimum temperature at which substantial hydrolysis occurs without excessive sugar degradation. Overall, the differences in conversion among the three POMF sources were minimal, indicating that variations in the initial cellulose and hemicellulose contents did not significantly influence the extent of hydrolysis under the simulated steam-explosion conditions.

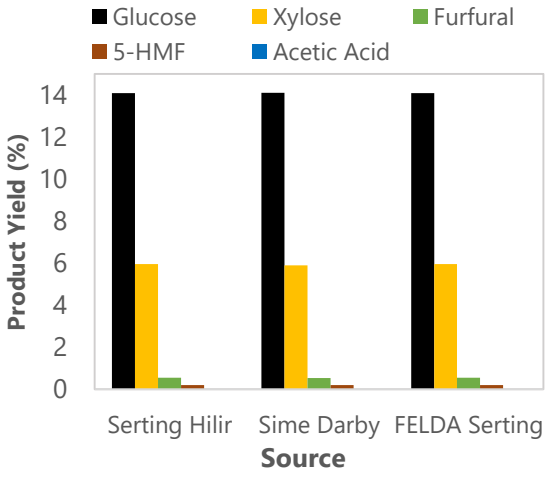


Fig. 6: Effect of POMF composition on product yields (T=150˚C, t= 3.5 min)

Effect of Temperature

Figure 7 illustrates the effect of steam explosion temperature on cellulose and hemicellulose conversions. Hemicellulose conversion increased markedly with temperature, rising from 87.5% at 110°C to nearly 100% above 160°C. In contrast, cellulose conversion was already complete (100%) at 110°C under the simulated conditions. Elevated temperatures enhance water autoionization and promote the release of acetyl groups, thereby increasing auto hydrolytic activity within the lignocellulosic matrix (Yang *et al.*, 2024). Consequently, higher temperatures accelerate the depolymerization kinetics of cellulose and

hemicellulose, facilitating their conversion into glucose and xylose, respectively (Nandiwale *et al.*, 2014).

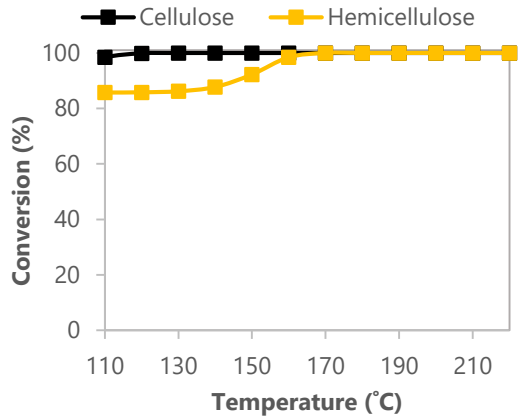


Fig. 7: Effect of steam explosion temperature on cellulose and hemicellulose conversions (POMF from FELDA Serting, t=3.5 min)

Figure 8 shows the effect of steam explosion temperature on product yields. All products exhibited strong temperature dependence. Glucose yield increased slightly from approximately 12.7% at 110°C to about 14.3% at intermediate temperatures, followed by a sharp decline as the temperature rose from 170 to 210°C. Xylose was not detected at 110°C but increased substantially from 0.47 to 10.1% as the temperature increased from 130 to 160°C, after which its yield decreased markedly at higher temperatures. These trends reflect the typical behavior of hydrothermal pretreatment, where hemicellulose and cellulose hydrolysis dominate at low-to-moderate temperatures. In contrast, while at elevated temperatures, released sugars become unstable and undergo secondary degradation reactions (Zhu *et al.*, 2023). Correspondingly, furfural production increased significantly above 160°C, reaching ~14.2% at 210°C, consistent with the accelerated acid-catalyzed dehydration of xylose at higher temperatures (Zhu *et al.*, 2023). A similar pattern was observed for 5-HMF, whose yield rose markedly between 170 and 210°C due to enhanced glucose dehydration under high-severity conditions (Azahanim *et al.*, 2019). Temperature, however, had no measurable effect on acetic acid formation within the investigated range.

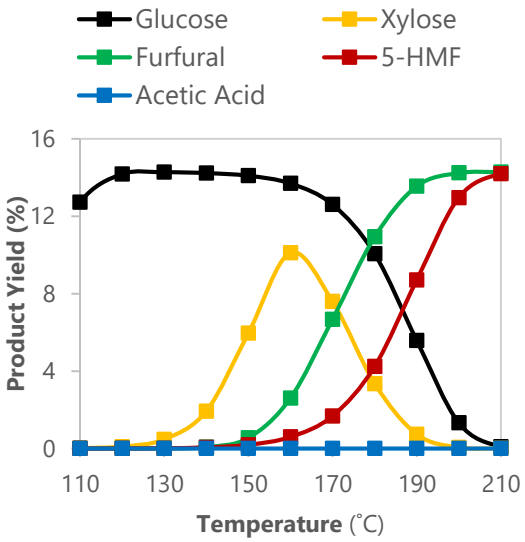


Fig. 8: Effect of reaction temperature on product yields (POMF from FELDA Serting, t=3.5 min)

Effect of Residence Time

Residence time is the duration the POMF is held at the target temperature before the rapid depressurization step that characterizes steam explosion. Figure 9 shows the influence of residence time on hemicellulose and cellulose conversions. Hemicellulose conversion increased steadily from 92% at 3.5 min to complete conversion (100%) at 10 min. In contrast, cellulose conversion was already complete at the shortest residence time evaluated (3.5 min) under the simulated conditions. Extending the residence time increases the overall severity of the steam explosion process. Prolonged exposure to hydrothermal conditions enhances autohydrolysis and promotes further depolymerization reactions for both

hemicellulose and cellulose (Ziegler-Devin *et al.*, 2021).

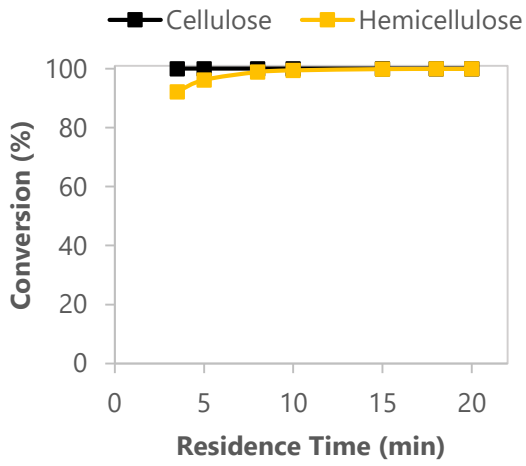


Fig. 9: Effect of residence time on cellulose and hemicellulose conversions (POMF from FELDA Serting, T=150˚C)

Figure 10 shows that glucose yield decreased markedly from approximately 14.1 to 2.3% as the residence time increased from 3.5 to 20 min. A similar trend was observed for xylose, whose yield declined to 1.4% at 20 min after initially forming at shorter residence times. In contrast, furfural yield increased slowly with residence time, indicating that extended exposure at 150°C promotes secondary degradation pathways. At this temperature, prolonged residence time imposes substantial stress on the system, leading to rapid sugar loss. The effect of residence time appears more severe than that of temperature. Both glucose and xylose become unstable under extended hydrothermal conditions and are increasingly converted into dehydration products. Xylose dehydration leads to higher furfural formation, while glucose follows a comparable but less pronounced pathway, producing elevated amounts of 5-HMF with increasing residence time. No acetic acid formation was detected within the studied range. These observations indicate that steam explosion requires short residence times to maximize sugar recovery while minimizing the formation of degradation products (Ziegler-Devin *et al.*, 2021).

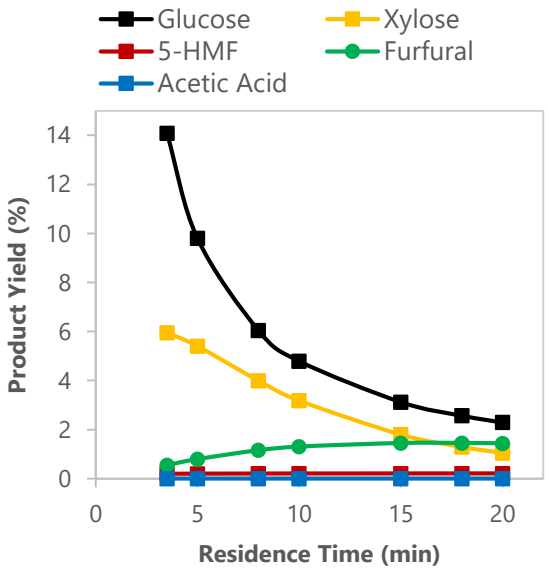


Fig. 10: Effect of residence time on product yields (POMF from FELDA Serting, T=150˚C)

CONCLUSIONS

In this study, the steam explosion of POMF was evaluated using the Aspen Plus® simulation platform. The process was modeled as a semi-batch operation employing the RBatch reactor model (R-103). The steam explosion temperature strongly influenced both sugar yields and the product formation. Glucose yield remained relatively stable at intermediate temperatures but decreased sharply as the temperature increased from 170 to 210°C. Xylose followed a similar pattern, increasing up to 160°C before declining substantially at higher temperatures. Correspondingly, the formation of degradation products such as furfural and 5-HMF became increasingly pronounced above 160°C. Residence time exerted a greater effect than temperature, as prolonged exposure led to pronounced

degradation of both glucose and xylose and to increased production of furfural and 5-HMF. These results indicate that short residence times are essential to maximize sugar recovery while minimizing degradation. Overall, the simulation study effectively modelled the steam explosion behavior of POMF and enabled the identification of optimal operating conditions of the steam explosion process.

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