

SYNERGISTIC ENHANCEMENT OF AROMATIC COMPOUNDS VIA CO-PYROLYSIS OF POLYURETHANE WASTE AND COCONUT SHELLS

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Abstract

This study investigates the enhancement of pyrolytic oil quality and fuel properties from polyurethane (PU) waste through co-pyrolysis with coconut shells (CS), chosen for their abundance, high calorific value, and low ash content. PU and CS were co-pyrolyzed at different ratios (4:1, 3:1, and 2:1), alongside pyrolysis of the pure materials for comparison. Thermal properties of the feedstocks, prepared in the same proportions as the actual pyrolysis systems, were characterized and used to construct decomposition models via the Criado plot method. Co-pyrolysis (PUCS) produced liquid yields (30.2–35.5 wt%) lower than theoretical values (40.4–42.6 wt%), indicating secondary decomposition reactions that converted condensable vapors into gases, likely promoted by PU–CS interactions. GC/MS analysis revealed that co-pyrolysis significantly enhanced the selectivity toward aromatic compounds (74.9–79.7%) through synergistic effects, facilitated by deoxygenation, hydrogen transfer, and Diels–Alder reactions. The highest aromatic compounds selectivity was observed at a PU:CS ratio of 3:1 (PUCS_3,1), indicating the strongest synergistic effect at this ratio. Moreover, the co-pyrolysis reduced the oxygen content of the pyrolytic oils attributed to higher degree of deoxygenation. Therefore, reduced oxygen content and increased aromatic carbon contributed to higher heating values (HHVs), demonstrating that PU–CS co-pyrolysis can yield improved-quality fuels from mixed waste and biomass feedstocks.

Keywords: Aromatic compounds; Coconut shells; Co-pyrolysis; Polyurethane waste

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Introduction

Polyurethane (PU), commonly used in foam form, is one of the most widely used polymers, with applications spanning various industries including construction, sports equipment, automotive, furniture, and mattresses (Font *et al.*, 2001). PU is synthesized via a polymerization reaction in which a polyol (a compound containing multiple hydroxyl groups) reacts with a diisocyanate (an organic compound with reactive isocyanate –NCO groups) in the presence of a catalyst. Consequently, PU consists of two distinct segments in its molecular structure: soft segments from polyols, and hard segments, from diisocyanates and chain extenders. The ratio and type of these segments determine the physical and mechanical properties of PU (Ristić *et al.*, 2023).

PU is difficult to recycle because its polymer networks are held together by strong covalent bonds that do not easily break down when heated (Karulf *et al.*, 2025). Traditional disposal methods such as landfilling and incineration can lead to serious environmental issues, including the release of hazardous substances and greenhouse gases such as hydrogen cyanide (HCN) and nitrogen oxides (NO_x), and CO₂. Therefore, pyrolysis—a thermal decomposition process conducted under low or oxygen-free conditions—which can reduce the formation of harmful gases presents a highly promising approach for the recycling of polyurethane (PU) materials (Ni *et al.*, 2024).

The pyrolysis of PU for oil production has been previously investigated, revealing that it generates oils with unique characteristics due to PU's high nitrogen content and complex polymer structure. These oils can serve as a source of specialty chemicals such as amines and pyrazoles (Chen *et al.*, 2023a). Nevertheless, the pyrolysis of PU also poses disadvantages due to the potential release of hazardous emissions—even under low-oxygen conditions—and the formation of toxic nitrogen-containing byproducts (Xu *et al.*, 2024).

Co-pyrolysis of PU with biomass can help dilute hazardous emissions and tailor the composition of pyrolytic products. In fact, two main methods are commonly employed to upgrade the quality of pyrolytic oil: catalytic pyrolysis (using catalysts) and co-pyrolysis (blending different feedstocks). Co-pyrolysis is generally simpler and more flexible than catalytic pyrolysis, as it does not necessarily require specialized catalysts or post-treatment steps, making it more scalable and economically attractive.

In the case of co-pyrolysis of waste polymers with biomass, it offers a dual solution by addressing

waste management challenges in both municipal and agricultural sectors. The feedstock ratio also plays a crucial role in determining the decomposition reaction pathways during co-pyrolysis (Nardella *et al.*, 2022).

In co-pyrolysis studies involving polyurethane (PU), various types of biomass have been employed, including wheat straw (Ni *et al.*, 2025), sawdust and palm leaf (Patcharavorachot *et al.*, 2024), corn stover (Li *et al.*, 2025), and almond shells (Aamir and Hassan, 2025). Nevertheless, to the best of our knowledge, the co-pyrolysis of coconut shells and polyurethane waste has not been thoroughly investigated to date.

Coconut shells are the hard, protective outer layer (endocarp) of the coconut fruit and are considered a form of agricultural waste, generated in large quantities worldwide. They can be classified as a type of hardwood due to their high density, mechanical strength, high lignin content, and low ash content—characteristics comparable to traditional woody biomass (Watcharawitthaya *et al.*, 2024).

The higher lignin content promotes the formation of aromatic hydrocarbons (AHs) and long-chain aliphatic species, whereas the lower ash content ensures stable operation and minimizes reactor fouling. Among hardwood biomass, lignin structures vary considerably. In coconut shells, guaiacyl (G) units dominate, resulting in highly condensed aromatic rings and the generation of stable phenoxy radicals, which in turn promote greater AHs production (Latif *et al.*, 2022). These characteristics make coconut shells more advantageous than the previously studied materials (non-wood: wheat straw, palm leaf, and corn stover; hardwood: almond shells and sawdust).

Coconut shells have been employed in co-pyrolysis processes to improve system efficiency, even when combined with other biomass types. Coconut shells (with low ash content) have been blended with rice husk (high ash content) in co-pyrolysis systems, and it has been found that increasing the proportion of coconut shells in the blend enhances the decomposition rate during co-pyrolysis (Kazawadi *et al.*, 2022).

Co-pyrolysis of coconut shells with plastics such as polypropylene (PP) and high-density polyethylene (HDPE) is also of great interest. Evaluation of activation energy reveals that the pyrolysis of coconut shells occurs in the range of 187.84–199.31 kJ/mol, while plastics exhibit a broader range between 169.15 and 360.04 kJ/mol (Rambhia *et al.*, 2025). Thus, coconut shells

represent a promising biomass feedstock that can enhance process efficiency and support the development of sustainable energy production from agricultural waste.

Criado's master plot method is a valuable analytical tool for investigating the thermal decomposition mechanisms of various materials, including biomass and polymeric wastes (Agnihotri and Mondal, 2024). This method relies solely on data obtained from thermogravimetric analysis (TGA), making it highly practical for pyrolysis studies. By comparing the normalized experimental decomposition rate with theoretical curves derived from different solid-state kinetic models, the Criado method enables the identification of the most probable reaction mechanism governing thermal degradation.

Therefore, in this study, the co-pyrolysis of waste polyurethane (PU) and coconut shells (CS) was investigated. The feedstock ratios of PU to CS were varied at 4:1, 3:1, and 2:1 to evaluate the effect of composition on the pyrolysis behavior. For comparison, the individual pyrolysis of pure PU and pure CS was also conducted under identical conditions. To gain insights into the thermal degradation mechanisms, the Criado's master plot method was employed, constructed from thermogravimetric data. The chemical compositions of the resulting pyrolytic oils were characterized using gas chromatography coupled with mass spectrometry (GC/MS). Furthermore, the synergistic effects between PU and CS were assessed based on the yield and selectivity of key valuable components—particularly aromatic compounds—produced during the co-pyrolysis process.

Materials and Methods

Materials

Polyurethane residues (PU) were provided by Karnyang Yeen Yong Industry Limited Partnership, Samut Prakan, Thailand. Coconut shells (CS) were sourced from a local market in Nakhon Pathom, Thailand. PU was ground into powder, while CS was washed, dried, and ground into particles approximately 10 mm in size. Both materials were oven-dried at 105°C for 24 h and then stored in a desiccator for further use.

Characterization of Feedstocks

Proximate and ultimate analyses were conducted for both polyurethane (PU) and coconut shell (CS) samples. The proximate analysis was carried out using TGA to determine moisture, volatile matter, fixed carbon, and ash content.

The ultimate analysis was performed with a CHNS analyzer following an in-house method based on ISO 16948:2015, which quantifies the elemental composition including carbon (C), hydrogen (H), nitrogen (N), and sulfur (S). For TGA, sample masses of 10–20 mg were analyzed under a nitrogen (N₂) ultra-high purity (UHP) atmosphere. The temperature was ramped from 25°C to 500°C at a heating rate of 10°C/min, and then held at 500°C for 1 h to ensure complete decomposition.

Activation energy of decomposition reactions were determined using the Coats-Redfern method, which provides a linearized form of the Arrhenius equation, adapted for non-isothermal conditions. For a reaction order of $n=1$, the equation simplifies to:

$$\ln \left[-\frac{\ln(1-\alpha)}{T^2} \right] = \ln \left[\frac{A}{(\beta E_a)} \right] - E_a/RT \quad (1)$$

where α is the degree of conversion or fractional weight loss, A is the pre-exponential factor, E_a is the activation energy, T is the absolute temperature in Kelvin, R is the universal gas constant (8.314 J/mol·K), and β is the heating rate in K/min.

The data obtained from thermogravimetric analysis (TGA) was also utilized to construct the Criado master plots, a model-fitting approach used to determine the reaction mechanisms involved in solid-state thermal decomposition processes. This method is based on the normalized rate function, as shown in Equation (2) (Criado *et al.*, 1989).

$$y(\alpha) = \frac{f(\alpha)}{f(\alpha)_{\max}} \quad (2)$$

where α is the degree of conversion, $f(\alpha)$ is the reaction model function, and $f(\alpha)_{\max}$ is the maximum value of the reaction rate function during decomposition.

$$\alpha = \frac{W_0 - W_t}{W_0 - W_f} \quad (3)$$

where W_0 is the initial mass of the sample (at the start of the TGA curve), W_t is the mass at time t during the thermal decomposition, and W_f is the final mass of the sample (at the end of the TGA curve). The reaction rate function, $f(\alpha)$, is then estimated using numerical differentiation of the TGA data, typically by calculating the derivative of mass loss with respect to temperature.

$$f(\alpha) = \frac{d\alpha}{dT} \quad (4)$$

From the calculation, the experimental data was plotted and compared with theoretical model-based master plots to determine the most suitable kinetic mechanism for the thermal decomposition. The models considered are:

F1: First-Order Reaction Model

$$f(\alpha) = (1 - \alpha) \quad (5)$$

This model assumes that the rate of conversion is directly proportional to the amount of unreacted material, which is common for many simple decomposition reactions. It implies a random and uniform breakdown of the solid matrix without significant diffusion or nucleation effects.

R3: Contracting Sphere Model

$$f(\alpha) = 3(1 - \alpha)^{2/3} \quad (6)$$

This model describes a reaction mechanism where the thermal decomposition progresses inward from the outer surface of a spherical particle toward its center. The rate of conversion is governed by the shrinking unreacted core – hence the term contracting sphere.

D3: Diffusion-Controlled 3D Model

$$f(\alpha) = \frac{3}{2}(1 - \alpha)^{\frac{2}{3}} [1 - (1 - \alpha)^{1/3}]^{-1} \quad (7)$$

This model assumes that the rate-controlling step is diffusion of gaseous products or reactive species through a solid product layer that surrounds the shrinking core of unreacted material.

Pyrolysis

Feedstock samples used in the pyrolysis experiments included pure polyurethane (PU), pure coconut shells (CS), and co-pyrolysis mixtures of PU and CS in weight ratios of 4:1 (PUCS_4,1), 3:1 (PUCS_3,1), and 2:1 (PUCS_2,1). The pyrolysis and co-pyrolysis experiments were conducted in a 5-liter stainless steel batch reactor equipped with a nitrogen (N₂) gas purging system to maintain an inert atmosphere throughout the process.

The heating protocol involved a constant heating rate of 10°C/min, ramping from room temperature to 500°C, followed by isothermal holding at 500°C for 1 h. This ensured sufficient time for complete thermal decomposition of the feedstock. The nitrogen flow served to prevent oxidation and facilitate the removal of volatile pyrolysis products from the reaction chamber.

Characterization of Pyrolytic Oil

The chemical composition of the pyrolytic oil was analyzed using gas chromatography–mass spectrometry (GC–MS). The instrument used was a Thermo Scientific GC–MS system equipped with a TG-5MS capillary column coated with polyethylene glycol (PEG), with a length of 30 m, an internal diameter of 0.25 mm, and a film thickness of 0.25 μm. The conditions used were as follows: injection volume of 0.2 μL, oven at 40°C (1 min) and continued with heating rate of 10°C/min to 300°C, split mode with a ratio of 100:1 and injection temperature of 290°C. The compound composition was further used to determine the oxygen content and to calculate the higher heating value (HHV) using the following Boie formula (Ferdinand *et al.*, 2012):

$$HHV \left(\frac{MJ}{kg} \right) = 0.329C + 1.428H - 0.128O + 0.515N - 0.037S \quad (8)$$

where C, H, O, N and S are the mass percentages of carbon, hydrogen, oxygen, nitrogen and sulfur, respectively in the pyrolytic oils.

Synergistic Effect Evaluation

The synergistic interaction between polyurethane (PU) and coconut shells (CS) during co-pyrolysis was evaluated by comparing experimental values with theoretical values. The theoretical values represent expected outcomes based on a linear additive rule without any synergistic or antagonistic effects. The theoretical value of any considered parameter (e.g., product yield, compound content, etc.) was calculated using the following equation:

$$Y_{theoretical} = \omega Y_{PU} + (1 - \omega) Y_{CS} \quad (9)$$

where $Y_{theoretical}$ is the theoretical values of the parameter (product yields and compound contents), ω is the mass fraction of PU in the blend, and Y_{PU} and Y_{CS} are the experimental values of the parameter of pure PU and CS.

Results and Discussion

Characterization of Feedstocks

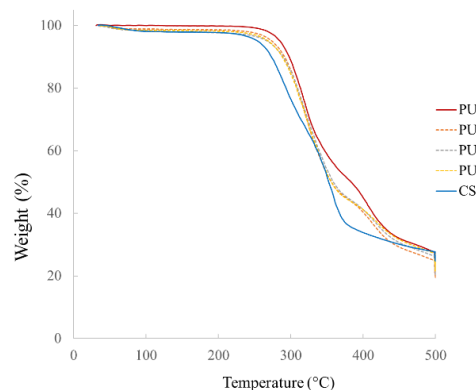
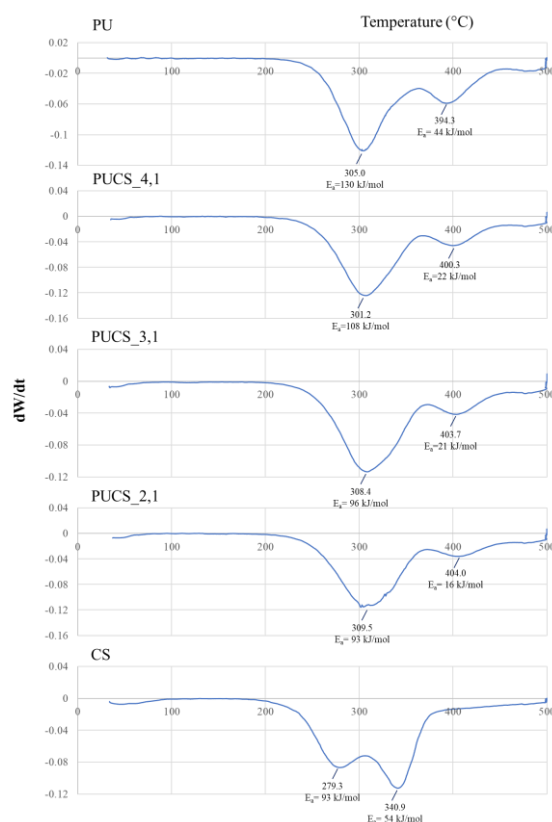
Polyurethane foam (PU) and coconut shells (CS), the feedstocks used for co-pyrolysis, were characterized using proximate and ultimate analyses. The analysis results are shown in Table 1. PU has high volatile matter and no ash, whereas CS has relatively high moisture content and a small

Table 1. Proximate and ultimate analysis of polyurethane (PU) and coconut shell (CS) feedstocks

Sample	Proximate analysis (wt%)				Ultimate analysis (wt%)			
	Moisture content	Volatile matter	Fixed carbon	Ash	Carbon (C)	Hydrogen (H)	Nitrogen (N)	Oxygen (O)
PU	0.13	83.02	16.85	0	65.76	6.49	7.14	20.61
CS	5.06	73.50	20.27	1.17	50.17	5.86	0.37	43.60

amount of ash. This could lead to a higher liquid yield from PU than from CS, and a lower char yield (Jiao *et al.*, 2013). In addition, high oxygen content in CS is observed as expected from biomass material. Therefore, oxygen-rich compounds are likely to be produced during the pyrolysis of CS, which could deteriorate the quality of the resulting liquid oil. Nevertheless, the co-pyrolysis of PU and CS is anticipated to produce synergistic effects and improve the quality of the oil.

Thermal property analysis of the feedstock was conducted using the TGA technique, which replicates the pyrolysis process on a microscale. The samples were heated at a rate of 10°C/min to 500°C and held at this temperature for 1 h. The TGA curves of the samples are presented in Figure 1. In addition, the DTG curves, which represent the rate of mass change as a function of temperature, are presented in Figure 2.

**Figure 1. Thermogravimetric analysis (TGA) curves of PU, CS, and PU–CS mixtures****Figure 2. Derivative thermogravimetric (DTG) curves of PU, CS, and PU–CS mixtures**

From Figure 1, PU exhibits two sharp decomposition stages, whereas CS shows a broader and more gradual decomposition profile typical of lignocellulosic biomass. CS retains the highest char residue (24.8 wt%), reflecting its high lignin content and naturally high fixed-carbon fraction. PUCS samples exhibit decomposition patterns that lie between pure PU and pure CS, showing clear synergistic interactions. They begin losing mass slightly earlier than PU, influenced by the thermally labile hemicellulose component in CS. The multistage decompositions in PUCS are also evident, consisting of an initial slope similar to PU, a merged mid-range decomposition region where PU and CS components degrade concurrently, and a tailing region (380–500°C) governed by the lignin-rich CS, which shows slower mass loss than pure PU.

From the DTG curves, PU exhibits a two-step thermal degradation process, as typical (Ismoilov *et al.*, 2019). The first stage (200–300°C) corresponds to the decomposition of urethane bonds, while the second stage (300–500°C) is attributed to the degradation of the more thermally stable polymer backbone. For CS, two broad DTG peaks are observed, indicating a multi-stage degradation process in which each stage may overlap across a wide temperature range. The first peak between 280–300°C is attributed to the decomposition of cellulose, and the second peak between 330–360°C corresponds to the decomposition of hemicellulose. Lignin, on the other hand, decomposes gradually over a much broader temperature range (approximately 250–600°C) due to its complex aromatic structure; as a result, its degradation is not clearly distinguishable in the DTG curves (Vamvuka *et al.*, 2003).

The DTG plots of all PUCS samples exhibited similar patterns, suggesting overlapping decomposition events of the two materials. The first broad peak around 300°C indicates a wider degradation profile, which may integrate the decomposition of both PU segments, and the cellulose and hemicellulose of CS. The presence of CS may also induce synergistic effects, such as facilitating the earlier degradation of PU and promoting radical recombination, thereby influencing the overall thermal degradation pathway (Uzoejinwa *et al.*, 2018). The second peak around 400°C could be attributed to the secondary degradation of lignin (Fenner and Lephardt, 1981), with interactions between PU and CS possibly creating conditions that promote these reactions, which are not clearly evident in the decomposition of pure CS.

Among the PUCS samples, the onset temperatures (T_{onset}) of the first DTG peak changed slightly, increasing with higher coconut shell content. Nevertheless, the activation energy (E_a)

evaluated around T_{onset} decreased with increasing coconut shell content. These observations may be attributed to catalytic interactions or synergistic effects that promote the degradation of PU, such as enhanced heat transfer, free radical interactions, and facilitated bond cleavage, thereby reducing the energy barrier for thermal degradation (Huang *et al.*, 2024).

Based on TGA/DTG data, the reaction mechanism of solid-state thermal decomposition processes can be determined using model-fitting methods that compare experimental data to various theoretical kinetic models. The Criado method is frequently used to analyze reaction mechanisms in co-pyrolysis, as it is specifically designed to address complex thermal decomposition behaviors. This method involves generating a master plot from experimental data and comparing it to theoretical plots derived from various kinetic models, providing the identification of the most appropriate reaction mechanism.

Common reaction models tested using the Criado method are shown in Figure 3, including F1 (first-order reaction), R3 (contracting sphere model), D3 (diffusion-controlled model), and A2 (Avrami–Erofeev nucleation model, $n = 2$).

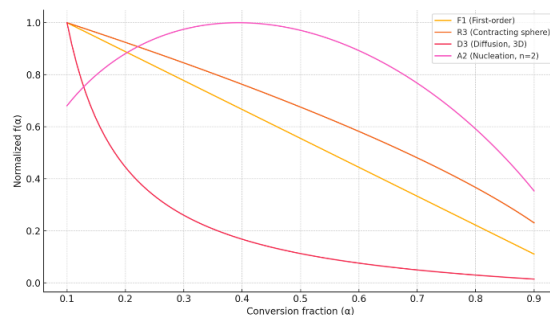


Figure 3. Criado master plots for selected reaction models (F1, A2, R3, and D3), illustrating theoretical conversion behaviors used for kinetic mechanism determination

The TGA/DTG data of all samples were used to calculate the conversion fraction (α) and the reaction rate function $f(\alpha)$, which were then plotted for comparison with the Criado master plots. It was found that A2 models closely fit the experimental data, as evaluated by the mean square error (MSE, ~ 0.1). The nucleation model (A2) provides a better fit for all samples, including CS—the pure biomass—despite diffusion models (such as D3) being more commonly applicable to biomass decomposition (Sobek and Werle, 2020). Therefore, the experimental data for all samples are

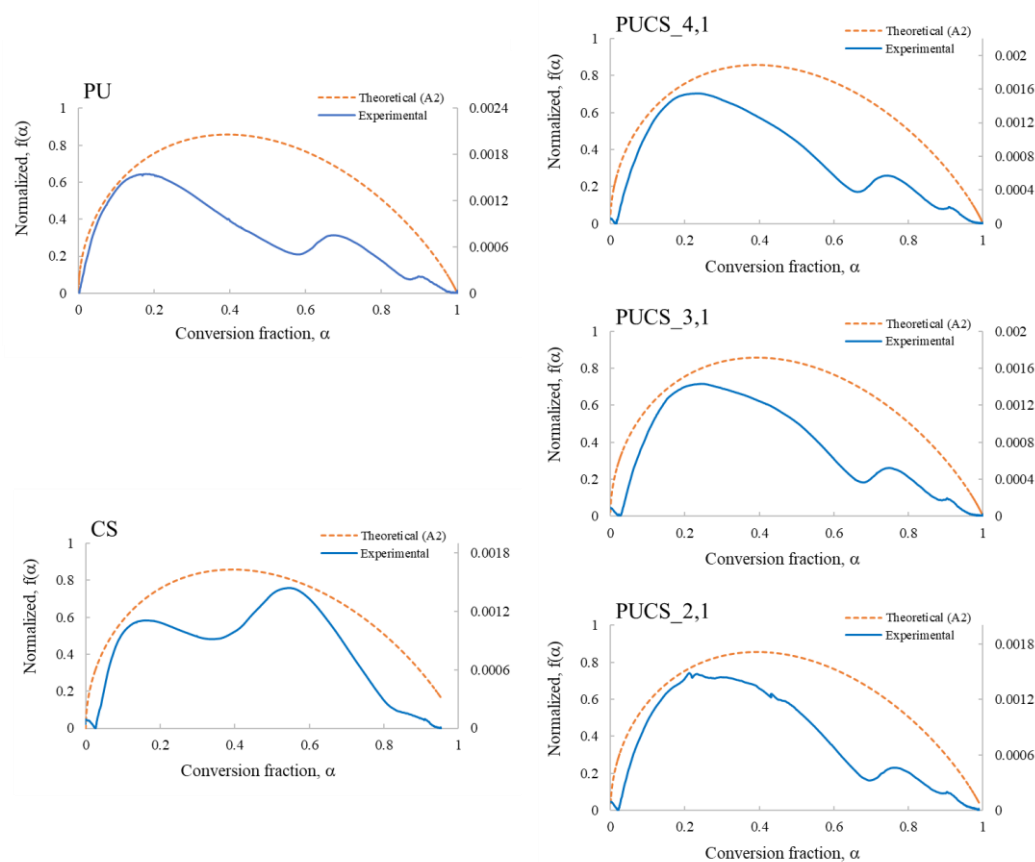


Figure 4. Criado master plots comparing experimental data of PU, CS, and PU–CS mixtures with the A2 nucleation model

compared with the nucleation model, as presented in Figure 4.

It can be seen that the nucleation model exhibits a sigmoidal (S-shaped) profile, indicating a low reaction rate at the early stage of conversion (α), followed by an increase to a peak in the middle stage, and a gradual decline thereafter. In fact, this is consistent with the degradation behavior of synthetic polymers like PU, which typically features three stages of decomposition (Vyazovkin *et al.*, 2011). It includes (1) an initial lag phase, where few nuclei are formed and the reaction rate is slow due to limited reactive sites; (2) an acceleration phase, during which the reaction rate increases as nuclei grow and the number of reactive centers expands; and (3) a deceleration phase, where the reaction rate declines as the reactants are gradually consumed.

Nevertheless, the experimental curve of PU deviated significantly from the theoretical A2 shape, suggesting multiple overlapping degradation processes. Therefore, the nucleation mechanism alone cannot adequately describe PU decomposition.

The additives within the polymer may inhibit complete degradation, and the conditions generated during pyrolysis may not sufficiently promote the decomposition process. Interestingly, the experimental curves of all PUCS samples exhibited closer conformity to the theoretical A2 model, indicating synergistic interactions between PU and CS during co-pyrolysis. This observation is likely because co-pyrolysis introduces heterogeneous PU–CS interfaces, mineral-active sites, and lignin-derived radical interactions that promote nucleation and subsequent two-dimensional growth of reaction fronts. These synergistic effects shift the degradation behavior from simple random scission toward nucleation-controlled kinetics.

For CS, the experimental curve exhibited a broader distribution with multiple peaks, suggesting complex, multi-step decomposition arising from its lignocellulosic structure (Burra and Gupta, 2019). The discrepancies between experimental and theoretical curves across all samples suggest that, although nucleation models offer a reasonable basis, the decomposition process is more accurately

described by a combination of mechanisms such as nucleation, diffusion, and random scission.

Variations in biomass content did not noticeably affect the kinetic model, as evidenced by the nearly identical A2 profiles among all PUCS samples, suggesting similar decomposition processes. Nevertheless, because multiple mechanisms operate simultaneously during pyrolysis, the dominant pathways may differ among the PUCS samples, resulting in variations in their compound distributions.

The scaled-up pyrolysis experiments, which produced sufficient quantities of products for reliable characterization, revealed distinct variations in compound distributions among all PUCS samples as well as between the PU and CS controls. These findings may correspond to the specific reaction pathways that predominate in each sample.

Pyrolysis

All samples with varying feedstock compositions were pyrolyzed in a pilot-scale batch reactor. The resulting products—condensable vapors, solid char, and non-condensable gases—were separated as follows: vapors were condensed (as liquid products) outside the reactor using a condensation system; solid char remained inside the reactor; and the non-condensable gases were released through

a treatment system without further analysis. The product yields from pyrolysis and co-pyrolysis of all samples are illustrated in Figure 5.

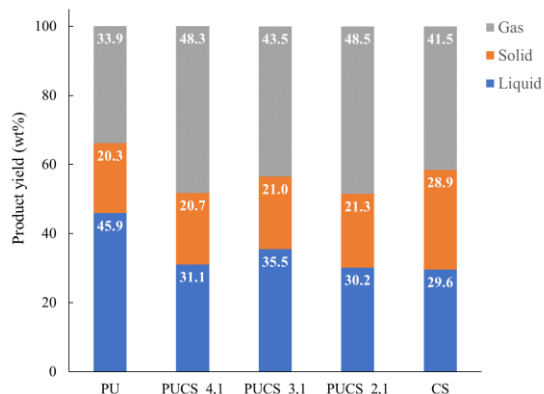


Figure 5. Distribution of product yields from the pyrolysis and co-pyrolysis of PU, CS, and PU–CS mixtures

Additionally, Figure 6 presents a comparison between the experimental yields and the theoretical yields of the co-pyrolysis systems (PUCS), calculated based on the pyrolysis results of pure PU and CS.

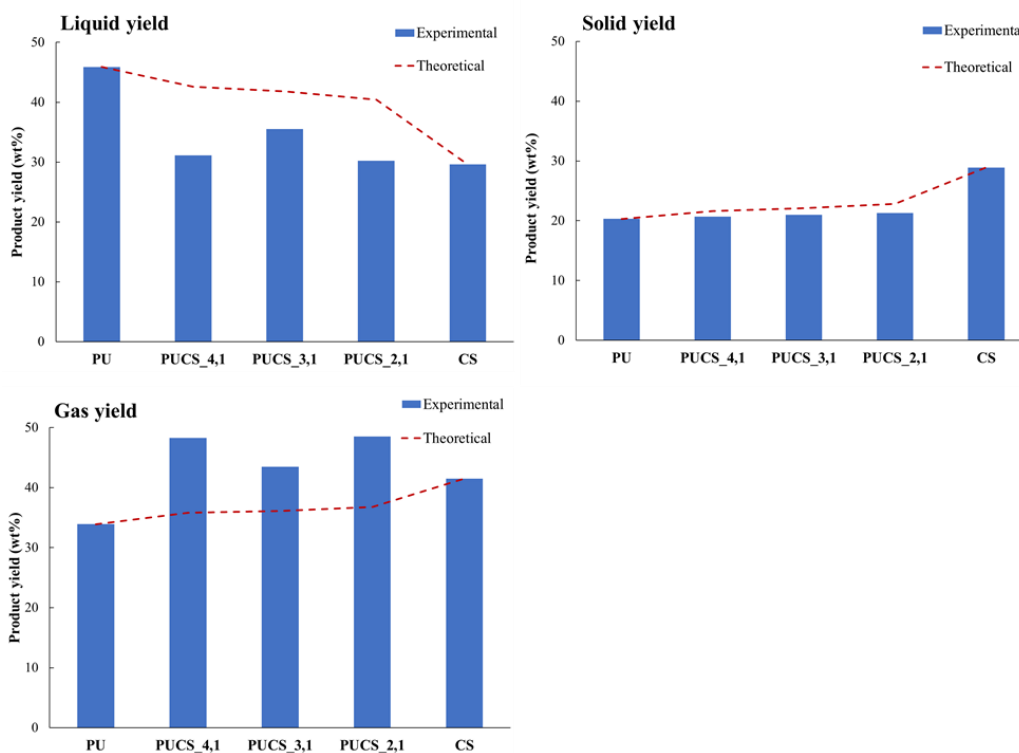


Figure 6. The experimental yields and the theoretical yields from the pyrolysis and co-pyrolysis systems

PU yields the highest oil (liquid) fraction, which is typical of synthetic polymers and can be attributed to its high volatile-matter content, whereas CS produces the highest gas yield due to the decomposition of lignocellulosic components—particularly hemicellulose and cellulose—which favor the formation of gas-phase products (El-Sayed *et al.*, 2024). Therefore, in the co-pyrolysis systems, the presence of CS is expected to decrease the oil yield while increasing the gas yield. The observed product yields align with this expectation. Nevertheless, as observed in Figure 7, the liquid yields for PUCS are lower and the gas yields are higher than the corresponding theoretical values. This suggests that secondary reactions, which convert liquid products into gas, are possibly promoted by interactions between PU and CS. The solid yield (char) reaches its highest value for pure CS, owing to its high fixed carbon and lignin content—both of which promote char formation. Across all co-pyrolyzed samples, the char yield remains relatively constant, ranging from 20.7 to 21.3 wt%. This implies that char formation is not significantly influenced by interactions between PU and CS.

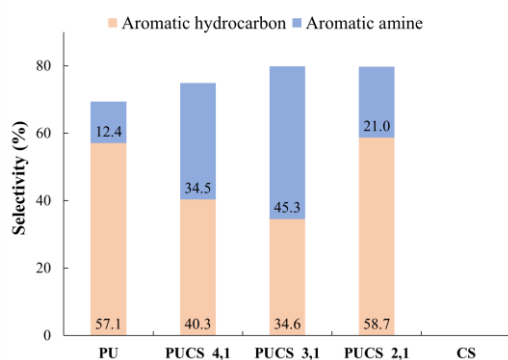


Figure 7. Selectivity toward aromatic compounds in pyrolytic oils obtained from PU, CS, and PU–CS mixtures

Characterization of Pyrolytic Oil

The resulting oils from all pyrolysis and co-pyrolysis systems (pyrolytic oils) were characterized by GC–MS to determine their chemical compositions, which help elucidate the reaction phenomena occurring during the pyrolysis of various feedstock mixtures. Figure 6 presents the selectivity toward aromatic compounds, including benzene, toluene, ethylbenzene, xylene (BTEX), and aniline, which were identified as the predominant compounds derived from the pyrolysis and co-pyrolysis of PU and PUCS, accounting for 69.4–79.7% of the total products.

The other compounds aside from aromatic compounds derived from PU and PUCS are presented in Figure 8, whereas the compounds obtained from the pyrolysis of CS, which are entirely different from those of the other samples, are shown in Figure 9.

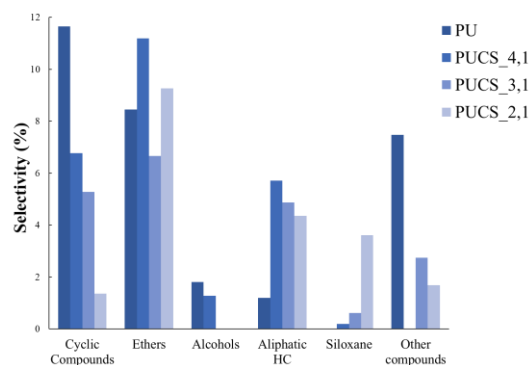


Figure 8. Selectivity toward non-aromatic compounds in pyrolytic oils obtained from PU and PU–CS mixtures

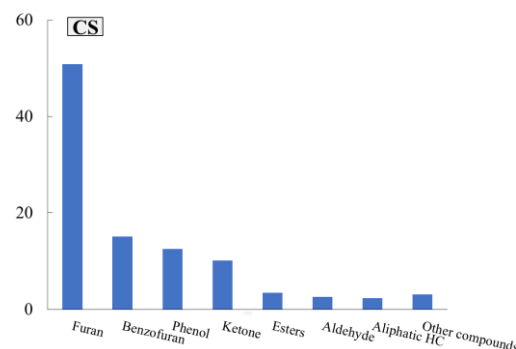


Figure 9. Selectivity toward various compound groups in pyrolytic oils derived from CS

It is observed that pure CS does not produce aromatic compounds to the same extent as PU or PUCS (excluding furan derivatives such as benzofuran and oxygenated compounds such as phenols). However, when CS is involved in the co-pyrolysis system with PU, it contributes to an increase in aromatic compounds selectivity. This increase is attributed to the appropriate chemical composition and synergistic thermal interactions between PU and CS during co-pyrolysis.

To better understand the synergistic effects between PU and CS, at first, the decomposition behavior of pure PU and CS, particularly the pathways involved in aromatic compounds

production, should first be described. Three primary mechanistic pathways have been proposed for the thermal decomposition of PU, (Hiltz, 2015): (PW1) dissociation of the urethane linkage into an isocyanate and an alcohol; (PW2) formation of a primary amine, an olefin, and carbon dioxide (CO₂) via a six-membered transition state; and (PW3) decarboxylation to yield a secondary amine, although the latter has not been shown due to a lack of supporting evidence.

As high amounts of aromatic compounds were observed in the pyrolysis products, it is likely that the isocyanate-based monomers used in the PU formulation consist of aromatic diisocyanates such as methylene diphenyl diisocyanate (MDI) and toluene diisocyanate (TDI). Thus, the expected products from the primary decomposition through two main pathways (PW1–2) should predominantly include aromatic isocyanates and amines, such as aniline, as illustrated in Figure 10.

Aromatic isocyanates can undergo decarboxylation to form aromatic amines and may also undergo bond-cleavage reactions that directly produce AHs (Li *et al.*, 2024). Aromatic amines can further undergo deamination, releasing NH₃ to form phenyl radicals, which subsequently rearrange into

AHs through processes such as aromatization, alkylation, and multiple substitutions. The alcohols and olefins generated from the polyol segments during the primary decomposition of PU could serve as hydrocarbon precursors for the aforementioned reactions.

Although the pyrolysis of pure CS in this study did not produce aromatic compounds, a plausible mechanism for their formation through biomass pyrolysis is still proposed in Figure 11, serving as a conceptual guideline for understanding the co-pyrolysis behavior of CS and PU.

The thermal decomposition of biomass begins with the primary degradation of its three main components. Among them, cellulose and hemicellulose primarily produce furan derivatives, while lignin—an abundant source of aromatic structures—contributes mainly to the formation of monocyclic phenols. From the analysis of pyrolyzed oil derived from CS, phenolic compounds, furans (especially furfural), and benzofuran were identified as the dominant constituents. This indicates that under non-catalytic pyrolysis conditions, CS primarily undergoes primary decomposition, leading to the formation of furan derivatives and phenolic compounds.

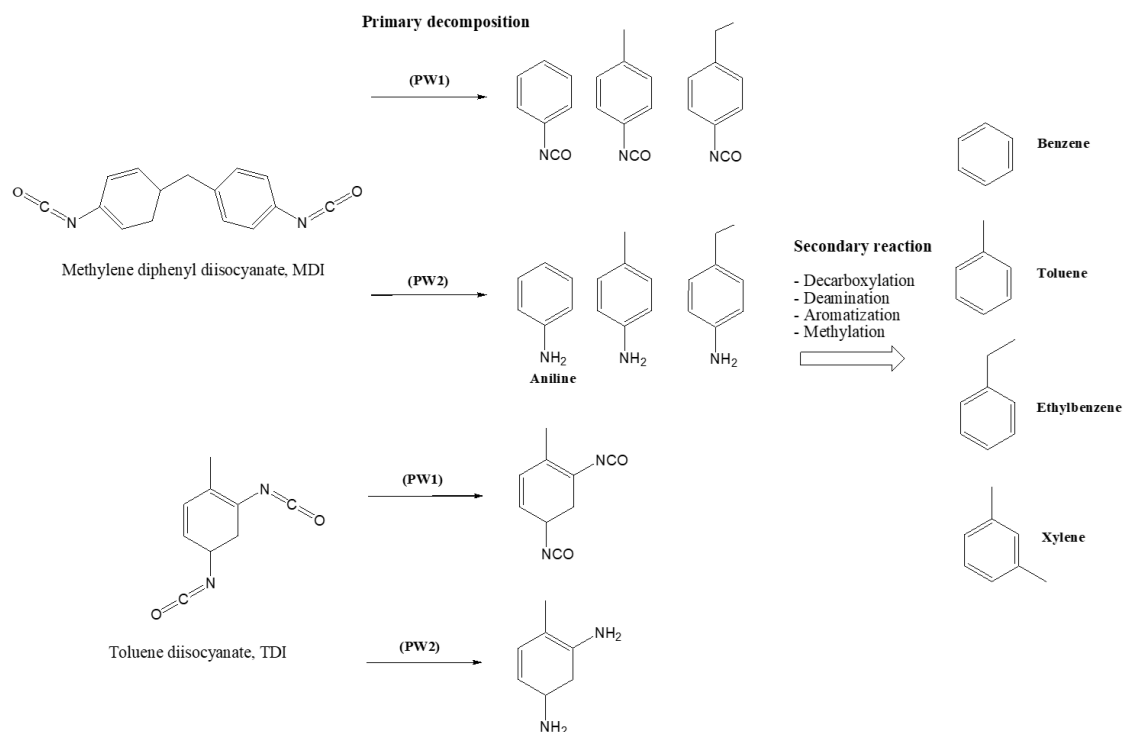


Figure 10. Proposed reaction pathways of methylene diphenyl diisocyanate (MDI) and toluene diisocyanate (TDI) during pyrolysis leading to the formation of aromatic compounds

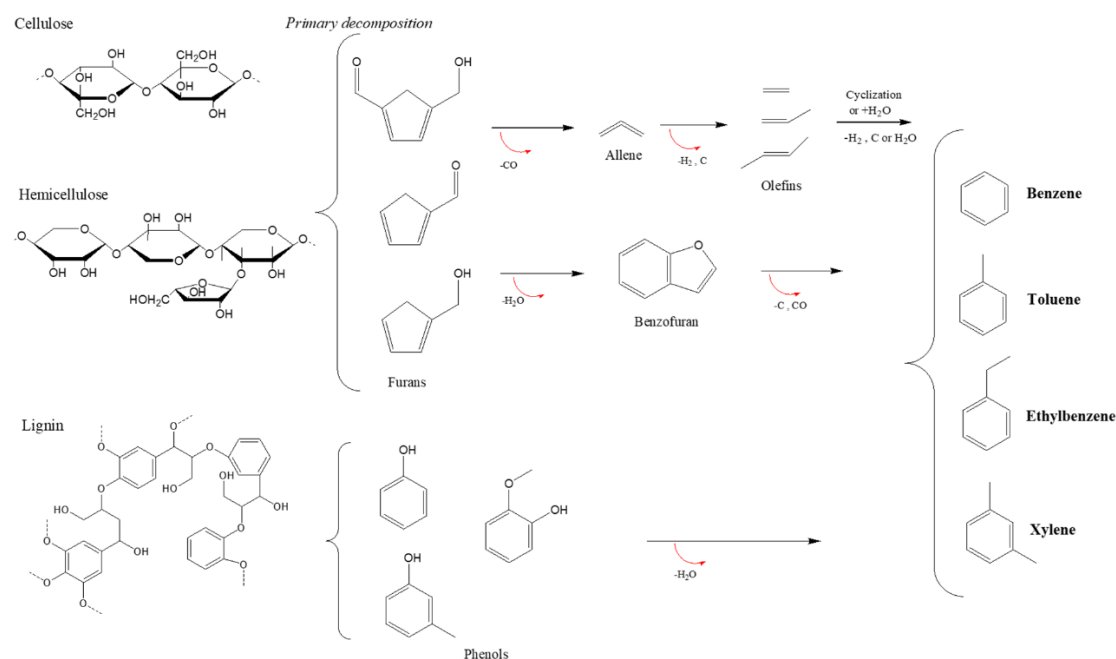


Figure 11. Proposed reaction pathways of lignocellulosic biomass during pyrolysis into aromatic hydrocarbons

Catalytic upgrading, particularly using shape-selective zeolites such as HZSM-5, is one method used to significantly enhance aromatization, promoting the transformation of intermediates such as furfural and benzofuran into benzene, toluene, and xylene (Osatiashiani *et al.*, 2022). Co-pyrolysis, as performed in this study, is also considered a viable method for upgrading pyrolysis systems.

As observed from the Criado method analysis, all PUCS samples exhibited synergistic effects between PU and CS during co-pyrolysis, introducing additional mechanisms not observed in the pure materials. In the co-pyrolysis, the PU-derived fragments (such as -NH and $\text{-CH}_2\text{-}$ groups) can act as hydrogen donors, stabilizing reactive intermediates from biomass (e.g., furans, phenols, and benzofuran). This hydrogen transfer facilitates deoxygenation processes (by releasing H_2O , CO , and CO_2) and promotes further secondary decomposition, as illustrated in Figure 11 (Akancha *et al.*, 2019). As a result, oxygenated biomass-derived intermediates tend to shift toward the formation of AHs rather than remaining as oxygenates. In addition, PU-derived hydrocarbon pools—comprising olefins and alcohols—enhance the production of AHs from CS through mechanisms such as the hydrocarbon pool mechanism, hydrogen transfer reactions, and Diels–Alder reactions,

thereby increasing the yield of AHs (Sun *et al.*, 2025).

On the other hand, CS enhances the production of AHs from PU by introducing more phenolic radicals—derived from phenol (Zhong *et al.*, 2016)—into the system. These radicals participate in further reactions that promote the formation of stable AHs, especially under the favorable conditions created by the synergistic interaction between PU and CS. CS also reduces the activation energy of decomposition, as observed earlier, leading to a faster overall pyrolysis process. This facilitates specific reaction pathways, such as reducing oxygen-containing compounds and promoting the formation of AHs.

Moreover, CS contributes to the accumulation of aromatic amines, particularly aniline, during co-pyrolysis. This effect can be attributed to two factors: the promotion of aniline formation and the suppression of its further transformation into secondary products (Figure 10).

The increased formation of aniline arises from synergistic char–vapor interactions, whereby CS-derived char catalyzes the conversion of isocyanates into aniline through surface reactions or acid–base catalysis (Chen *et al.*, 2023b). In addition, phenolic radicals generated from CS intermediates can directly react with amine species, thereby promoting the formation of aniline (Lardy *et al.*, 2019).

The reduction in aniline conversion occurs when CS-derived volatiles, particularly phenolics, act as hydrogen donors that stabilize PU-derived isocyanate fragments, thereby directing them toward aniline formation rather than secondary decomposition. This stabilization effect may also influence subsequent secondary reactions, favoring the production of AHs.

From the results, it can be concluded that at a moderate CS content (PUCS_3,1), the synergistic effect of CS on aniline formation is most pronounced. However, at a higher CS ratio (PUCS_2,1), this effect is diminished, while the enhancement of AHs formation becomes more pronounced. The higher amounts of phenolic radicals generated at high CS ratios may accelerate reactions that promote AHs formation.

High-aniline pyrolytic oil can serve as a valuable chemical feedstock for applications such as the reproduction of polyurethane (via MDI precursors), as well as in the manufacture of dyes and pigments, pharmaceutical intermediates, and rubber processing chemicals (Chaturvedi and Katoch, 2020). Furthermore, in co-pyrolysis with PU, high aniline yields can serve as an indicator of PU-derived synergy, reflecting the efficiency of PU decomposition. From the GC/MS data, both the oxygen content and higher heating value (HHV) of the pyrolytic oils were determined, as shown in Figure 12. It was observed that the oxygen content in the oils derived from the pyrolysis of pure PU and CS were 6.60 wt% and 24.01 wt%, respectively. Interestingly, the introduction of CS into the co-pyrolysis system resulted in a reduction in the oxygen content of the resulting oils. Moreover, this decreasing trend continued as the proportion of CS increased, with the following values: PUCS_4,1 (4.53%), PUCS_3,1 (3.27%), and PUCS_2,1 (2.82%).

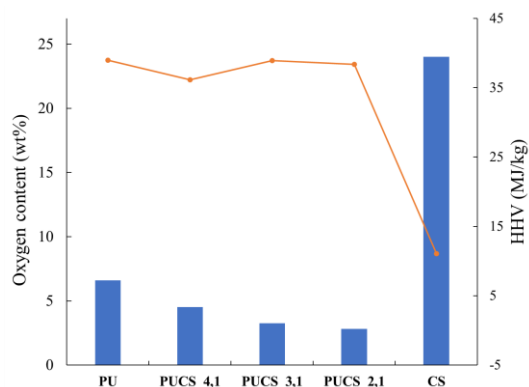


Figure 12. Oxygen content (blue bar) and HHV (yellow line) of pyrolytic oils obtained from PU, CS and PU–CS mixtures

Higher degrees of deoxygenation may occur due to the introduction of CS in the co-pyrolysis system. These deoxygenation pathways include dehydration, decarboxylation, and decarbonylation (removal of H₂O, CO₂, and CO), which are essential in reducing oxygen-containing compounds in the resulting oils. These reactions not only contribute to the oxygen removal but also promote the formation and selectivity of aromatic compounds. This is consistent with the observed increase in aromatic compounds production in the co-pyrolysis systems.

Nitrogen contents in the pyrolytic oils were also quantified, revealing that the co-pyrolysis systems produced higher nitrogen levels (3.32–6.11 wt%) compared with pyrolysis of pure PU (2.18 wt%), while CS itself contributed no nitrogen-containing compounds. This is attributed to the higher aniline content in the PUCS pyrolytic oils, indicating that most nitrogen-containing species remain in stable liquid forms rather than being further converted into toxic emissions such as NH₃, NO_x, or HCN.

A lower oxygen content in the pyrolytic oils improves fuel quality by minimizing oxidation reactions, which otherwise lead to the formation of undesirable polar compounds and free radicals that degrade the fuel's stability, calorific value, and storability (Gharby *et al.*, 2025). The increase in higher heating value (HHV) is also enhanced by the reduction in oxygen content. The HHV of oils derived from PU and PUCS co-pyrolysis ranges between 36.18–38.99 MJ/kg, while CS-derived oil exhibits the lowest HHV of 11.05 MJ/kg. This improvement in HHV is attributed not only to the lower oxygen content, which reduces energy-limiting oxygenated compounds, but also to the high contents of AHs, particularly BTEX, and aromatic amines such as aniline in PU and PUCS oils. These compounds possess high energy densities, thereby contributing to the superior fuel quality of the resulting oils.

It is observed that PUCS_3,1 produces pyrolytic oil with the highest HHV among all co-pyrolysis systems. In addition, it exhibits the highest selectivity toward overall aromatic compounds and aniline, and also yields the greatest amount of pyrolytic oil among all tested ratios. Therefore, a PU-to-CS ratio of 3:1 (PUCS_3,1) can be considered the optimum blending ratio for the co-pyrolysis of PU and CS.

Conclusion

Co-pyrolysis of polyurethane (PU) and coconut shells (CS) at different mixing ratios was carried out

to enhance the quality and fuel properties of pyrolytic oils. The results revealed that co-pyrolysis (PUCS) reduced liquid yields, even lower than the theoretical values, indicating secondary decomposition reactions that converted condensable vapors into gases, likely promoted by interactions between PU and CS. Importantly, co-pyrolysis enhanced the selectivity toward aromatic compounds through synergistic effects, facilitated by reactions such as deoxygenation, hydrogen transfer, and Diels–Alder cycloaddition. These reactions can be efficiently promoted by phenolic radicals generated from CS. The strongest synergistic effect was observed at a PU:CS ratio of 3:1 (PUCS_3,1), which yielded the highest selectivity for aromatic compounds and aniline. Furthermore, the deoxygenation reactions reduced the oxygen content of the pyrolytic oils, and together with the increased aromatic compounds content, resulted in high higher heating values (HHV), even though part of the feedstock originated from biomass.

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Author Contributions

Conceptualization, K.S., A.J., and E.C.; Methodology, K.S., A.J., and E.C.; Validation, K.S., A.J., and E.C.; Investigation, P.K. and J.S.; Formal Analysis, K.S., T.S., C.J., U.A., A.J., and E.C.; Resources, K.S., T.S., C.J., U.A., A.J., and E.C.; Writing – Original Draft, K.S. and E.C.; Writing – Review & Editing, E.C.; Funding Acquisition, K.S.

Ethics Statement

This study did not involve human participants, animals, or identifiable personal data. Therefore, ethical approval and informed consent were not required in accordance with the institutional and national research guidelines.

Declaration of Generative AI Use

The authors declare that no Generative AI tools were used in the preparation of this manuscript.

Conflict of Interest

The authors declare that they have no conflicts of interest relevant to this work.

Data Availability Statement

The data generated and analyzed during the current study are available from the corresponding author upon reasonable request.

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