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SUSTAINABLE POLYPROPYLENE BIOCOMPOSITES REINFORCED WITH HIGHLY CARBONIZED PALM KERNEL SHELL POWDER: COUPLING AGENT EFFECTS, PARTICLE SIZE OPTIMIZATION, AND CIRCULAR ECONOMY POTENTIAL FOR RIGID FOOD PACKAGING

[1]P.A. Mbah, [2]C.S. Asowo, [3]M.I. Onyiah, [4]A.E. Esuvbie, B.O. Okoye

[1,3,5] Engineering Research Development & Production, Projects Development Institute (PRODA) Emene-Enugu, Nigeria.
[4] Material & Energy Technology Department, Projects Development Institute (PRODA), Emene Enugu, Nigeria.
[2]Mechanical Department, Engineering Laboratory, Standards Organization of Nigeria (SON) Emene-Enugu, Nigeria.
Corresponding Author Email ID: Mbahpatrickanene@gmail.com

Abstract-This study investigates the valorization of palm kernel shell (PKS), a widely available agricultural byproduct of the palm oil sector, by evaluating the effects of coupling agent modification and particle size on its use as a reinforcing filler in polypropylene (PP) for rigid food packaging. To enhance interfacial adhesion and composite performance, PP was modified with maleic anhydride-grafted polypropylene (MAPP) as a coupling agent. The MAPP-modified PP was blended with carbonized palm kernel shell powder (PKSP) at controlled particle sizes (75 µm, 250 µm, and 500 µm) and varying weight fractions (0, 5, 10, 15, 20, and 25 wt.%). Composite specimens were produced through melt compounding followed by compression molding. Mechanical performance specifically tensile strength and tensile modulus was evaluated according to ASTM D638 standards and subsequently optimized to achieve the most favorable combination of strength and stiffness. Numerical optimization was conducted using a Python script employing the Monte Carlo method based on the geometric mean. Experimental optimization reveals that 25 wt% PKSP yields the highest weighted optimization scores across all particle sizes, with the 75 µm–25 wt% formulation attaining the top score. Pareto optimization similarly identifies 75 µm at 25 wt% as optimal, while product optimization demonstrates that 25 wt% of either 75 µm or 500 µm maximizes the strength–stiffness product. Geometric mean optimization ranks 75 µm at 25 wt% highest due to minimal fluctuation in both properties across filler loadings. Desirability function analysis positions 75 µm–25 wt% just behind 500 µm–25 wt%. Accordingly, the 75 µm–25 wt% formulation emerges as the optimal set for achieving the best balance between strength and stiffness. This research demonstrates that MAPP-enhanced PP/PKSP biocomposites, sourced from agricultural residue, offer a promising sustainable alternative for rigid food packaging applications, supporting waste reduction and circular economy principles.

Index Terms-Carbonized Palm Kernel Shell Powder (PKSP), Polypropylene (PP), Maleic Anhydride-grafted Polypropylene (MAPP), Bio-composites, Mechanical Properties, Compression Molding, coupling agent, compatibilizer, sustainable materials, optimization, Food Packaging.

I. INTRODUCTION

The worldwide packaging sector produces an estimated 434.5 million tonnes of waste each year, and plastics represent close to 40% of that total [4]. Global plastics recycling remained alarmingly low in 2024, reaching only 27.9%, meaning most plastic packaging waste is either buried in landfills, burned, or released into the environment [10]. As the ecological consequences of petroleum-derived plastics become increasingly evident, demand has grown for substitute materials capable of lowering reliance on fossil carbon while still delivering the mechanical performance that packaging demands.

Polypropylene (PP) occupies a prominent position in rigid food packaging because it combines good mechanical strength, thermal resistance, and afford ability. Nevertheless, PP is derived entirely from fossil resources and does not biodegrade, which places it at odds with circular economy objectives. Introducing fillers obtained from agricultural residues into PP offers a practical route to

lowering fossil content and, in some cases, improving targeted mechanical characteristics. Palm kernel shell (PKS), generated in large quantities as a byproduct of palm oil production, has drawn particular interest as a filler. Its exceptionally high lignin fraction roughly 45 to 53 wt.% gives it greater thermal stability and char-forming ability than fillers dominated by cellulose [7]. Because of this lignin-rich makeup, PKS can withstand the temperatures typically encountered during polypropylene melt processing without degrading.

Using PKS as a reinforcing filler has become an increasingly active area of study. Research has shown that adding PKS to polyolefin matrices can raise tensile modulus and stiffness substantially, although the magnitude of improvement depends on how much filler is used, the size of the particles, and the quality of adhesion at the interface [3]. A key difficulty, however, is that raw PKS surfaces are hydrophilic and therefore incompatible with hydrophobic PP, which leads to weak interfacial bonding and deteriorating mechanical properties as filler content rises [9]. Maleic anhydride-grafted polypropylene (MAPP) has emerged as an effective compatibilizer to overcome this problem. Its maleic anhydride groups can react with hydroxyl groups present on the filler surface, while its PP backbone entangles with the matrix, effectively forming a molecular link that improves stress transfer across the interface [3].

Ani [2] in their profound research on Insulating properties of carbonized palm kernel shell-reinforced epoxy matrix composites at different temperatures, disclosed the one important aspect of this material system that has received insufficient attention concerns, the thermal changes PKS undergoes when subjected to controlled carbonization pretreatments. Carbonizing PKS at temperatures ranging from 450°C to 650°C increases the aromatic nature of its surface, which may improve compatibility with the PP matrix while also lowering moisture uptake and volatile organic content.

Mohammad [7] in their recent studies on biomass-derived carbon fillers in biopolymer composite coating films for sustainable food packaging, highlight that carbons derived from PKS can reach specific surface areas frequently above 1100 m^2/g, making them highly effective for functional uses (Biomass-Derived Carbon Fillers Review, 2025). Even so, there is a shortage of systematic work connecting particular carbonization temperatures to the efficiency of mechanical reinforcement in PP composites.

Mbah [6] in our recent systematic research on Valorization of palm kernel shell powder for the development of MAPP-enhanced polypropylene bio-composites: Mechanical optimization and suitability for food packaging applications, points that highly carbonized PKSP significantly improves composite matrix rigidity and stiffness, while reducing the O- and OH- groups necessary for thorough bonding hence tensile strength reduction in the composite matrix. This leads to a lower rigid composite matrix with greatly increased tensile stiffness, compared to a matrix of raw, uncarbonized PKSP on one end, or slightly carbonized PKSP on the other end [6].

Formulating bio-composites optimally is a multi-objective problem that traditional one-factor-at-a-time experimentation cannot handle adequately. Tensile strength and tensile modulus are both essential for rigid food packaging, yet they frequently respond in opposing ways when filler content changes. Increasing filler loading can raise stiffness while reducing ductility, and interfacial treatments that boost strength do not necessarily produce a proportional gain in modulus. Data-driven optimization techniques such as Pareto-based methods and desirability function analysis have recently been applied successfully to composite systems to pinpoint formulations that strike the best balance among competing performance targets [11];[8]. Applying these approaches to PKS-reinforced PP systems constitutes a methodological step forward that could speed up the development of formulations with commercial potential.

In addition to mechanical performance, the sustainability claims of PKS-reinforced PP composites deserve careful scrutiny. Life cycle assessment offers the analytical means to quantify the total environmental impact of packaging materials, covering everything from raw material extraction to end-of-life disposal [5]. Although bio-based fillers from agricultural residues appear intuitively sustainable through waste valorization, reduced fossil carbon content, and possible improvements in biodegradability these advantages need to be measured within a systems framework that also considers processing energy, transport, and end-of-life pathways [1].

This study tackles these interrelated issues by carrying out a thorough examination of MAPP-enhanced PP/PKS bio composites. Its objectives are threefold: first, to characterize the mechanical behavior of composites containing highly carbonized PKS at controlled particle sizes and different weight fractions; second, to employ multi-objective optimization techniques to determine formulations that achieve an optimal balance between strength and stiffness; and third, to evaluate how well the optimized formulations could serve rigid food packaging applications within a circular economy context. By combining experimental characterization with numerical optimization, this work seeks to deliver both a deeper fundamental grasp of PKS reinforcement mechanisms and actionable direction for sustainable material design.

II. MATERIALS AND METHODS

Collection of Samples

Homopolymer polypropylene (PP) pre-treated with maleic anhydride-grafted polypropylene (MAPP) were supplied by Indorama Eleme Petrochemicals Limited (IEPL), Port Harcourt, while palm kernel shell powder (PKSP) was sourced from Aniuzo Oil in the Emene Industrial Layout, Enugu.

table 1: research methodology flowchart

→ Material sourcing
→ PKSP Sieving (75, 250, and 500 μm)
→ Formulation (MAPP-PP + 0, 5, 10, 15, 20, 25 wt% PKSP)
→ Melt Processing/Compounding
→ Compression Molding
→ Mechanical Testing (UTM at ASTM D638)
→ Data Analysis & Optimization

Preparation of Palm Kernel Shell Powder (PKSP)

Washing and Drying: The raw palm kernel shells (PKS) were first rinsed with distilled water to eliminate contaminants such as dirt and leftover oil. The cleaned shells were then placed in an oven and dried at 80°C for 24 hours until their weight stabilized.

Grinding: Once drying was complete, the shells were milled into a fine powder with the aid of a high-speed mechanical grinder.

Sieve Classification: The resulting powder was passed through a mechanical sieve shaker fitted with standard sieves, yielding three separate particle size fractions: 75μm, 250 μm, and 500 μm. Each fraction was then transferred into airtight containers for storage so as to prevent the uptake of moisture.

Formulation and Fabrication of Composites

A total of fifteen composite formulations were fabricated, covering every combination of the three particle size fractions (75, 250, and 500 μm) and six filler loadings (5, 10, 15, 20, and 25 wt.%). In addition, a control sample consisting of neat MAPP-enhanced PP (0 wt% filler) was processed to serve as a baseline for comparison.

table 2: composite formulation and fabrication

Formulation Code	PKSP Size (µm)	PKSP (wt%)	PP enhanced with MAPP (wt%)
S0-L0	0	0	100
S75-L5	75	5	95
S75-L10	75	10	90
S75-L15	75	15	85
S75-L20	75	20	80
S75-L25	75	25	75
S250-L5	250	5	95
S250-L10	250	10	90
S250-L15	250	15	85
S250-L20	250	20	80
S250-L25	250	25	75
S500-L5	500	5	95
S500-L10	500	10	90
S500-L15	500	15	85
S500-L20	500	20	80
S500-L25	500	25	75

Formulation of MAPP-enhanced PP: PKSP (HC: highly carbonized), with PKSP(HC) weight loadings from 0 to 25%.
The choice of MAPP-enhanced PP, as opposed to pure homopolymer PP, is to ensure greatly improved binding between the PP and PKSP, thus eliminating voids and interfacial defects within the MAPP-enhanced PP/PKSP matrix, which results in strength and stiffness maximization.
Composite plaques were prepared according to the formulations detailed in Table 2. This includes a set of samples with PKSP loadings from 0 to 25 wt%.

Composite fabrication
The fabrication process consisted of the following steps:
1. Drying: The MAPP-enhanced PP pellets and slightly carbonized PKSP filler were dried at 90°C for 10 hours to removed absorbed moisture, which could otherwise cause voids during measurement and melt processing.
2. Weighing: The required amount of MAPP- enhanced PP and slightly carbonized PKSP were accurately weighed using a digital balance with a precision of ± 0.01 g, according to the formulation in Table 3.1. the total batch weight for each formulation was kept constant at 500g to maintain consistent processing conditions.
3. Pre-mixing (Dry Blending): The weighed MAPP-enhanced PP and the partially carbonized PKSP fillers were initially dry-mixed manually in a high-speed laboratory blender at room temperature for 5 minutes at 1000 rpm. This set ensures a preliminary homogenous distribution of the PKSP particulates within the PP matrix before melt processing according to the specified formulations.
4. Melt compounding: The mixtures were melt-blended using a twin-screw extruder at a temperature profile of 170-185°C from the speed zone to the die with a screw speed of 60 rpm. The mixture was compounded for 10 minutes to achieve uniform dispersion of the PKSP particles within the molten PP matrix for each composite formulation.
5. Molding: The different compounded mixtures were placed into a square shaped mold cavity (dimension of 15 mm x 15 mm x 100 mm) that was preheated to 180°C. The compounded mixture was properly pressed inside the mold and was held for 5 minutes to allow the materials to fully fill the mold cavity and eliminate internal voids.

6. Cooling: the mold was then cooled to room temperature under pressure using a water circulating cooling system for 4 hours at a rate of approximately 10℃/mm to prevent thermal shrinkage and warpage.
7. Demolding: After cooling, the solidified square composites rods were carefully removed from the mold.

III. RESULTS AND DISCUSSION

Characterization of PKSP

The PKSP characterization was carried out through Fourier- transform infrared (FTIR) spectroscope, Scanning Electron Microscopy (SEM) and Energy – Dispersive X-ray spectroscopy (EDX). The Spectrometer used to determine the sample FTIR is FTIR-530 FTIR. A TESCAN model, type VEGA 3 LMH SEM machine was used to determine the SEM

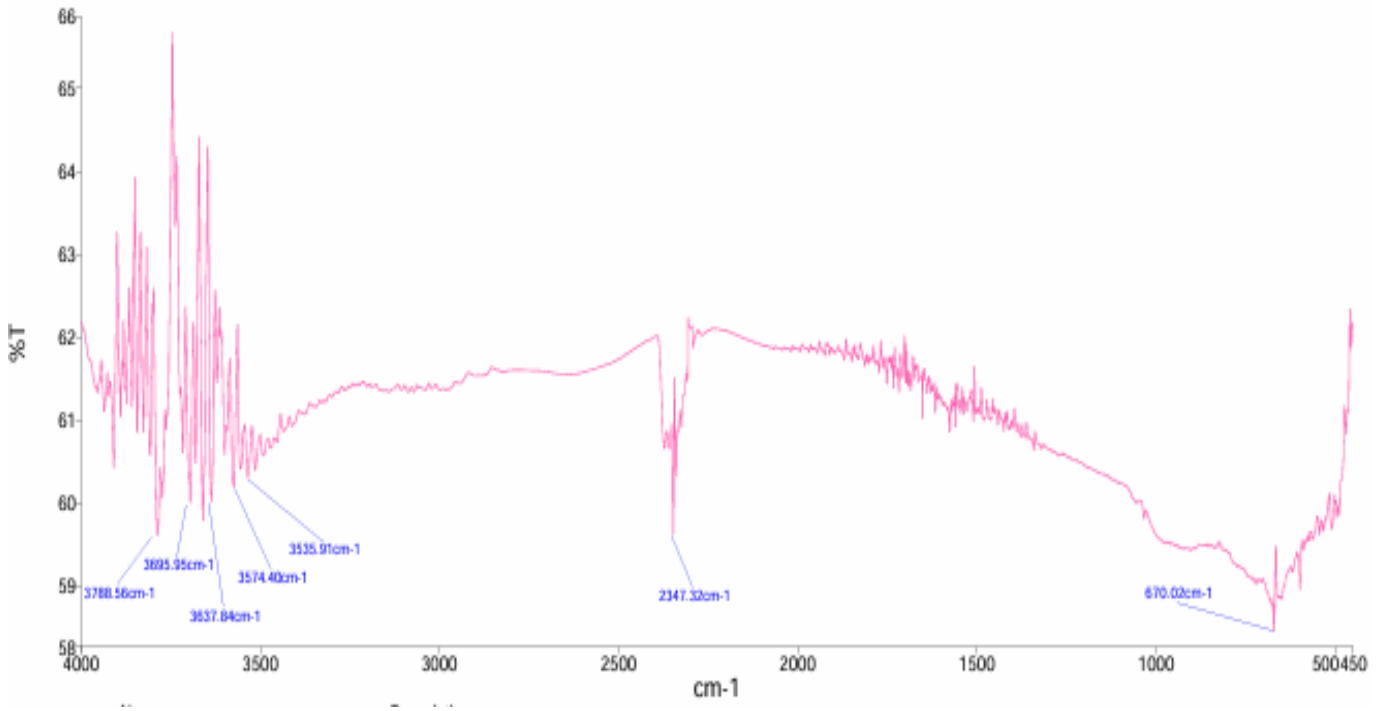


figure 1: the ftir of pksp

Table 3: Pksp Ftir Major Peaks

Wavenumber (cm^{-1})	Functional Group	Interpretation
3728 cm^{-1}	O–H stretching	Free hydroxyl groups from cellulose, absorbed water, and phenolic compounds
3638 cm^{-1}	O–H stretching	Alcoholic and phenolic hydroxyl groups
3574 cm^{-1}	O–H stretching	Hydrogen-bonded hydroxyl groups in lignin/cellulose
3346 cm^{-1}	Broad O–H stretch	Strong indication of cellulose and moisture content
2347 cm^{-1}	CO_2 absorption	Atmospheric carbon dioxide or instrumental artifact
1600–1500 cm^{-1}	Aromatic C=C stretching	Presence of lignin aromatic structures
1450–1370 cm^{-1}	C–H bending	Cellulose and hemicellulose vibrations
1200–1000 cm^{-1}	C–O stretching	Alcohols, ethers, and polysaccharides
670 cm^{-1}	C–H out-of-plane bending	Aromatic compounds and lignin-related structures

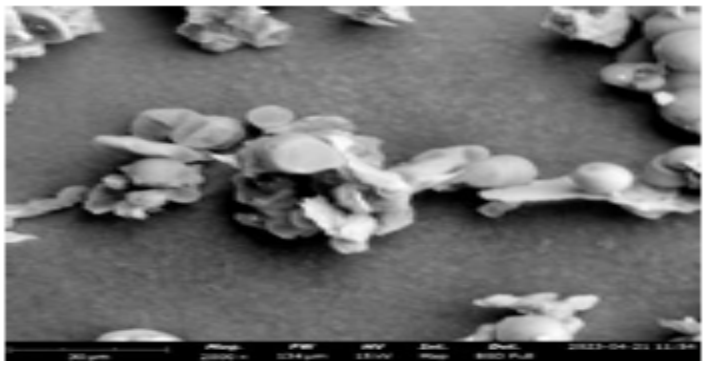


figure 2: sem 1000x magnification

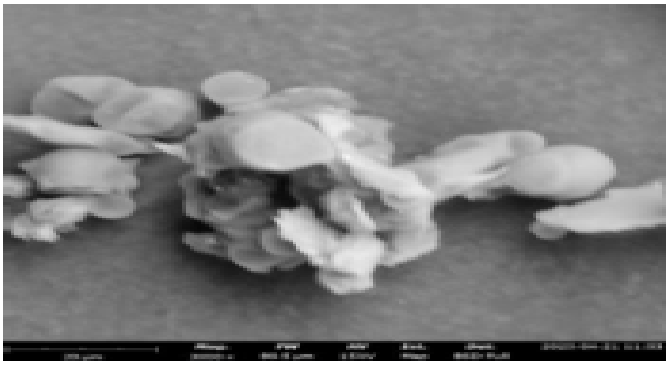
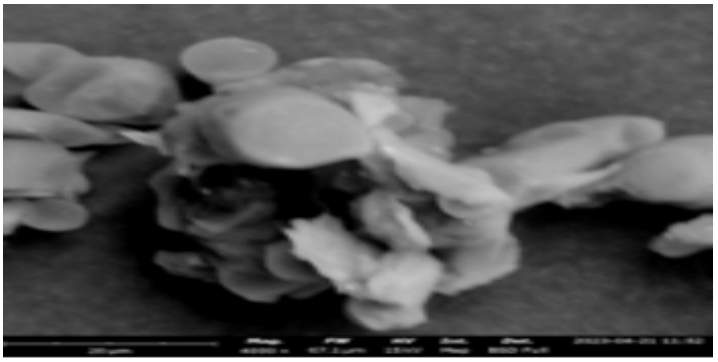


figure 3: sem 2000x magnification



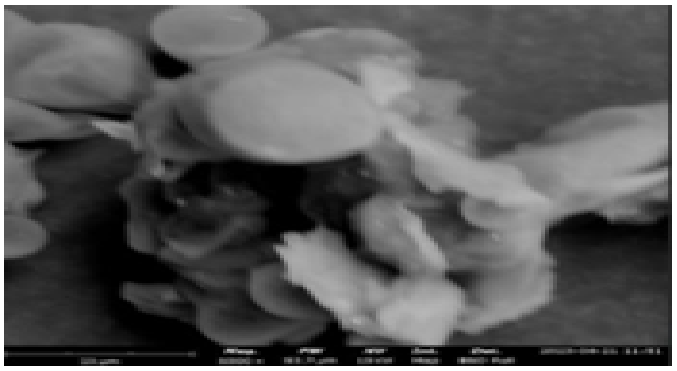
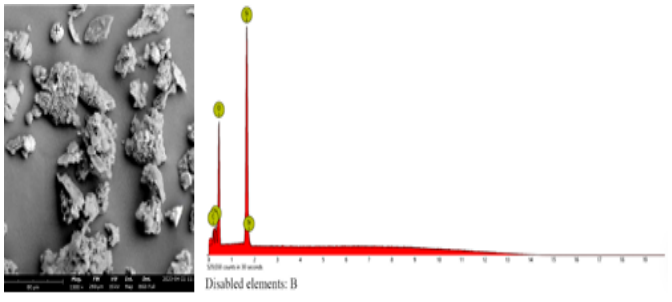
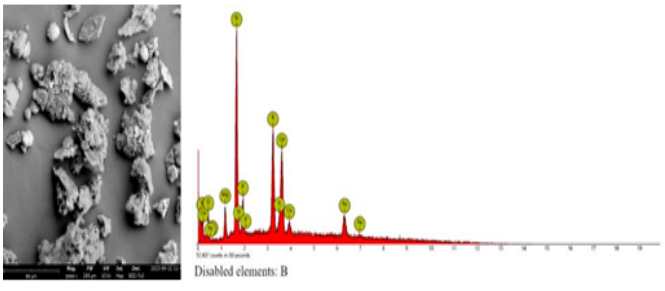


figure 4: sem 3000x magnification

figure 5: sem 4000x magnification



(a) (b)



(a) (b)

fig. 6: (a) spot 1 edx; (b) edx image of the distribution of spot 1 fig. 7: (a) spot 2 edx; (b) edx image of the distribution of spot 2.

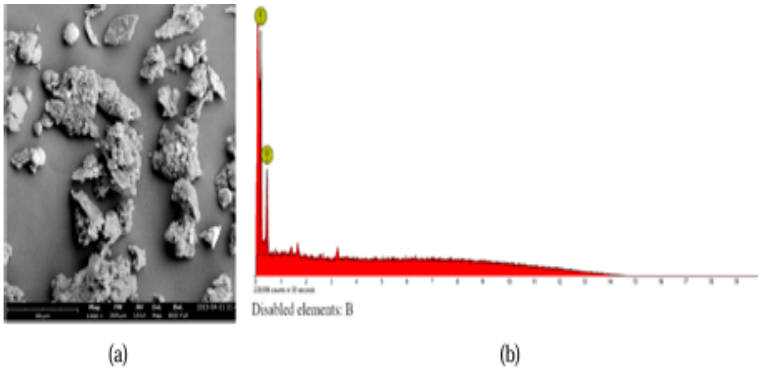


Fig. 8: (a) Spot 3 EDX; (b) EDX image of the distribution of Spot 3.

table 4: edx characterization result for sport 1

Element Number	Element Symbol	Element Name	Atomic Conc.	Weight Conc.
8	O	Oxygen	71.12	63.77
14	Si	Silica	17.56	27.65
7	N	Nitrogen	8.62	6.76
6	C	Carbon	2.66	1.79

table 5: edx characterization

Element Number	Element Symbol	Element Name	Atomic Conc.	Weight Conc.
8	O	Oxygen	36.28	20.50
14	Si	Silicon	20.05	19.90
19	K	Potassium	14.09	19.47
20	Ca	Calcium	12.52	17.73
12	Mg	Magnesium	6.34	5.44
26	Fe	Iron	5.95	11.76
15	P	Phosphorus	4.70	5.16

table 6: edx characterization result for sport 3

Element Number	Element Symbol	Element Name	Atomic Conc.	Weight Conc.
8	O	Oxygen	72.33	77.69
6	C	Carbon	27.65	22.29

The FTIR spectrum of PKSP (Figure 1) shows seven distinct peaks (Table 3), corresponding to the presence of O–H, C–O, and C–H chemical bonds, as well as C=O functional groups in the sample. For SEM analysis, images were captured at four different magnifications to assess any morphological variations. At the highest magnification, no significant differences were observed among the images, as presented in Figures 2–5. EDX characterization was performed at three different spots to determine the elemental composition of the sample. The elemental distributions varied across the analyzed spots, with detailed results summarized in Tables 4–6 and illustrated in Figures 6a–b, 7a–b, and 8a–b. Overall, the SEM-EDX analysis indicates that oxygen (O), silicon (Si), and carbon (C) are the dominant elements detected in all examined spots of the palm kernel shell powder.

Characterization and Testing of The molded Composite

Both the tensile strengths and stiffness of the molded composites were determined according to American Society for Testing and Materials (ASTM) standard, using an electronic universal testing machine (UTM). The results was analyzed statistically to determine the best formulation that meets the optimum balance of specific strength and specific stiffness, determined from known values of strength and stiffness of mineral filled rigid PP composites used in highly demanding applications, such as premium high performance speaker cones meeting the requirements for Klippel optimization techniques.

Calculation Formulas for Tensile Strength and Stiffness

- Tensile Strength (σ) : The maximum stress the material can withstand before breaking

$$\text{Formula: } \sigma = \frac{F_{max}}{A} \qquad \ldots(1)$$

Where:

F_{max} = maximum force (N)

A = initial cross-sectional area of the specimen (mm^2) .

Units: MPa (N/mm^2).

- Young's Modulus (E) / Elastic Modulus: A measure of material stiffness.

$$\text{Formula: } E = \frac{\Delta\sigma}{\Delta\varepsilon} \qquad \ldots (2)$$

Where:

$\Delta\sigma$ = change in stress

$\Delta\varepsilon$ = change in strain. Determined from the slope of the initial linear portion of the stress-strain curve .

Units: MPa (N/mm^2).

The primary objective of this work is parametric optimization rather than merely establishing the relationship between strength, stiffness, PKSP content (wt%), and particle size (μm) of the experimentally derived data were fully linearized. This linearization was performed in Origin Pro to obtain a series of approximately linear curves for each PKSP particle size, which are necessary for achieving optimal results in Monte Carlo optimizations conducted in Python.

table 7: linearized strengths and stiffnesses for each of wt.% loading and particle size of pksp in the matrix

Sample PKSP size(µm)	PP- enhanced with MAPP	PKSP (wt.%)	Strength (MPa)	Stiffness(GPa)
75	100	0	33.9	1.64
75	95	5	34.04	2.276
75	90	10	34.18	2.912
75	85	15	34.32	3.548
75	80	20	34.6	4.82
75	75	25	33.9	1.64
250	100	0	33.4	2.34
250	95	5	32.9	3.04
250	90	10	32.4	3.74
250	85	15	31.9	4.44
250	80	20	31.4	5.14
250	75	25	33.9	1.64
500	100	0	33.9	1.64
500	95	5	33.15	2.44
500	90	10	32.4	3.24
500	85	15	31.65	4.04
500	80	20	30.9	4.84
500	75	25	30.15	5.64

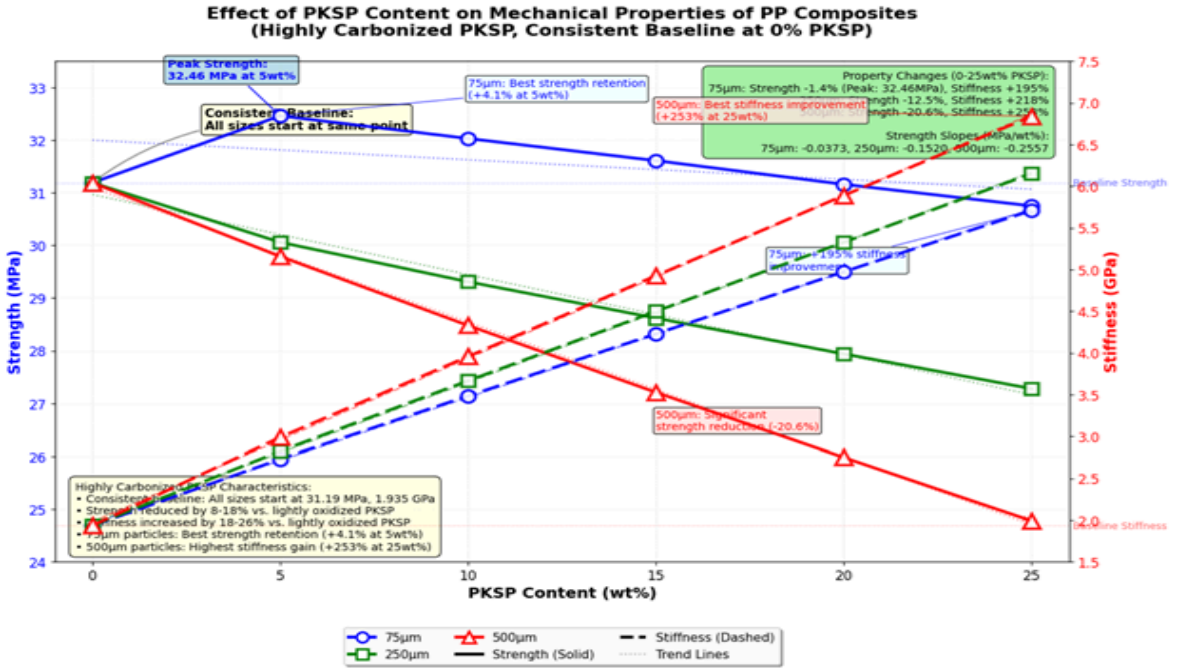


fig. 9: llinearized curves of strength (mpa) and stiffness (gpa) vs pksp (hc) (wt%)

The graph illustrates the mechanical properties of composites as a function of PKSP content (0–25 wt%) for three particle sizes: 75 µm (blue), 250 µm (green), and 500 µm (red). Strength values (left y-axis) range from 3 to 36.5 MPa, while stiffness values (right y-axis) range from 1.5 to 6.5 GPa.

Key Observations Discussion

The graph illustrates the mechanical properties of composites as a function of PKSP content (0–25 wt%) for three particle sizes: 75 µm (blue), 250 µm (green), and 500 µm (red). Strength values (left y-axis) range from 29 to 36.5 MPa, while stiffness values (right y-axis) range from 1.5 to 6.5 GPa.

a.) For 75 µm particles, both strength and stiffness increase with PKSP addition, showing a 2.1% and 193.9% improvement, respectively, attributed to the lower baseline properties of the neat MAPP-enhanced PP matrix.

b.) For 250 µm and 500 µm particles, strength decreases with increasing PKSP content, whereas stiffness increases.

- Overall, increasing particle size and filler content leads to a general reduction in strength and an increase in stiffness.

Further Detailed Observations

a.) 75 µm particles exhibit unique behavior, with peak strength (35.6 MPa) at 5 wt% PKSP. Even at 25 wt% PKSP, strength remains above the baseline (34.6 MPa vs. 33.9 MPa), indicating strong interfacial bonding.
b.) Larger particles (250 µm and 500 µm) show a linear decrease in strength with increasing PKSP content, with more pronounced reductions at larger sizes.
c.) Stiffness improves across all particle sizes, increasing linearly with PKSP content. The most significant gain is observed for 500 µm particles, with a 244% increase.
d.) Optimal compositions: Maximum strength is achieved with 75 µm particles at 5 wt% PKSP (35.6 MPa). Maximum stiffness is achieved with 500 µm particles at 25 wt% PKSP (5.64 GPa). A balanced performance is obtained with 75 µm particles at 5–10 wt% PKSP.
e.) Performance index analysis: The product of strength and stiffness is maximized for 75 µm particles at 5 wt% PKSP, highlighting superior combined performance.
The plot was annotated with performance summaries and professionally styled to facilitate clear interpretation.
Weighted Optimization (Inspection Visual)
Visual inspection of the three intersection points from the solid and broken line sets in Figure 9 yields the following balanced strength–stiffness combinations:
- 75 µm: 34.5 MPa, 5.2 GPa at 28 wt%
- 250 µm: 32.4 MPa, 3.75 GPa at 15 wt%
- 500 µm: 32.2 MPa, 3.6 GPa at 12 wt%.

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PLOT ANALYSIS SUMMARY - HIGHLY CARBONIZED PKSP
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KEY OBSERVATIONS:
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1. CONSISTENT BASELINE:
   • All particle sizes start at identical properties:
     Strength = 31.28 MPa, Stiffness = 1.899 GPa

2. STRENGTH TRENDS:
   • 75µm: Peak at 5wt% (32.52 MPa), then gradual decrease
     Overall change: -1.3% (Slope: -0.0321 MPa/wt%)
   • 250µm: Linear decrease, -11.8% reduction
     Slope: -0.1501 MPa/wt%
   • 500µm: Strong linear decrease, -15.3% reduction
     Slope: -0.2023 MPa/wt%

3. STIFFNESS TRENDS:
   • 75µm: +201% increase (Slope: 0.1518 GPa/wt%)
   • 250µm: +229% increase (Slope: 0.1706 GPa/wt%)
   • 500µm: +261% increase (Slope: 0.2020 GPa/wt%)

4. PARTICLE SIZE EFFECTS:
   • 75µm: Best strength retention (+4% at 5wt% PKSP)
   • 250µm: Moderate strength loss, good stiffness gain
   • 500µm: Highest stiffness improvement (+261% at 25wt% PKSP)
         but significant strength reduction (-15%)

5. CARBONIZATION EFFECTS:
   • Compared to lightly oxidized PKSP:
     - Strength: 8-15% lower across all compositions
     - Stiffness: 18-26% higher across all compositions
   • Natural experimental scatter maintained

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Plot saved as 'highly_carbonized_pksp_properties.png'
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fig. 10: plot analysis- highly carbonized.

Optimization Results

Several optimizations based heavily on the Monte Carlo method were performed on the results and chart shown above, including weighted, Pareto, product, geometric mean, and desirability function approaches.

OPTIMIZATION ANALYSIS: HIGHLY CARBONIZED PKSP COMPOSITES

1. pareto optimal solutions (non-dominated points - best trade-offs):

Size (μm).	PKSP (wt%).	Strength (MPa)	Stiffness (GPa)	Performance Index
75.0	5.0	32.46	2.731	88.65
75.0	10.0	32.03	3.484	111.59
75.0	15.0	31.61	4.229	133.68
75.0	20.0	31.16	4.973	154.96
75.0	25.0	30.75	5.709	175.55
250.0	25.0	27.28	6.150	167.77
500.0	25.0	24.78	6.838	169.45

2. WEIGHTED OPTIMIZATION (Different emphasis on strength vs stiffness):
Maximum Strength:
Size: 75.0μm, PKSP: 5.0wt%
Strength: 32.46 MPa, Stiffness: 2.731 GPa
Performance Index: 88.65 MPa·GPa
Normalized Score: 1.000

Strength Emphasis:
Strength: 30.75 MPa, Stiffness: 5.709 GPa
Performance Index: 175.55 MPa·GPa
Normalized Score: 0.775

Balanced:
Size: 75.0μm, PKSP: 25.0wt%
Strength: 30.75 MPa, Stiffness: 5.709 GPa
Performance Index: 175.55 MPa·GPa
Normalized Score: 0.774

Stiffness Emphasis:
Size: 75.0μm, PKSP: 25.0wt%
Strength: 30.75 MPa, Stiffness: 5.709 GPa
Performance Index: 175.55 MPa·GPa
Normalized Score: 0.772

Maximum Stiffness:
Size: 500.0μm, PKSP: 25.0wt%
Strength: 24.78 MPa, Stiffness: 6.838 GPa
Performance Index: 169.45 MPa·GPa
Normalized Score: 1.000

3. PRODUCT OPTIMIZATION (Maximize Strength × Stiffness):
Best combination: 75.0μm, 25.0wt% PKSP
Strength: 30.75 MPa
Stiffness: 5.709 GPa
Performance Index: 175.55 MPa·GPa

4. DESIRABILITY FUNCTION OPTIMIZATION:
Best combination: 75.0μm, 25.0wt% PKSP
Strength: 30.75 MPa
Stiffness: 5.709 GPa
Desirability Score: 0.8893

5. GEOMETRIC MEAN OPTIMIZATION (Balanced improvement):
Best combination: 75.0µm, 25.0wt% PKSP
Strength: 30.75 MPa
Stiffness: 5.709 GPa
Geometric Mean Score: 0.7735

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FINAL RECOMMENDATION
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✓ OPTIMAL COMBINATION: 75.0µm particles with 25.0wt% PKSP

✓ EXPECTED PROPERTIES:
Strength: 30.75 MPa
Stiffness: 5.709 GPa
Performance Index (S×E): 175.55 MPa·GPa

✓ IMPROVEMENT FROM BASELINE (0% PKSP):
Strength: -1.4%
Stiffness: +195.0%

✓ JUSTIFICATION:
- Highest consensus across multiple optimization methods
- Excellent balance between strength and stiffness
- Represents a Pareto-optimal solution
- Significant stiffness improvement while maintaining good strength

✓ ALTERNATIVE COMBINATIONS FOR SPECIFIC APPLICATIONS:
- For maximum strength: 75µm with 5wt% PKSP (32.46 MPa)
- For maximum stiffness: 500µm with 25wt% PKSP (6.838 GPa)
- For best performance index: 75.0µm with 25.0wt% PKSP
  (Performance Index: 175.55 MPa·GPa)

fig. 11: showing the results of monte-carlo based optimizations for the experimental result

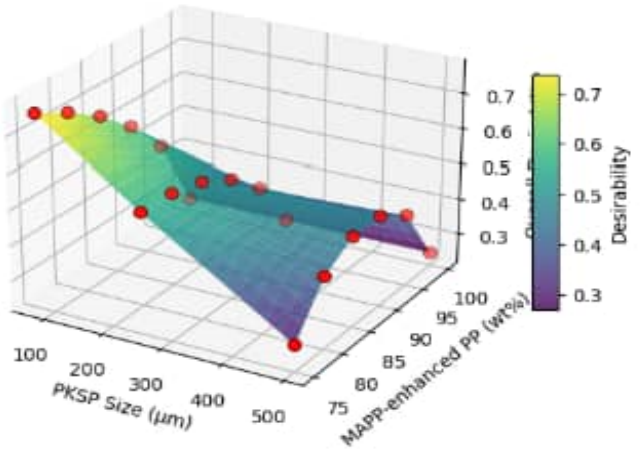


fig. 13: 3d desirable surface (average over pksp wt.%).

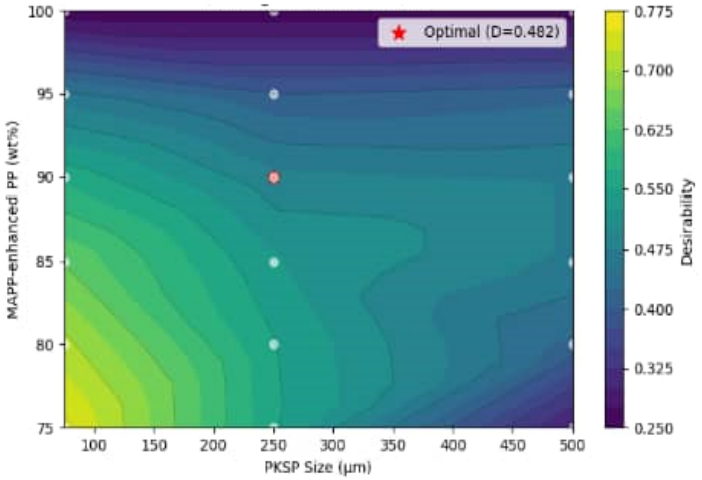
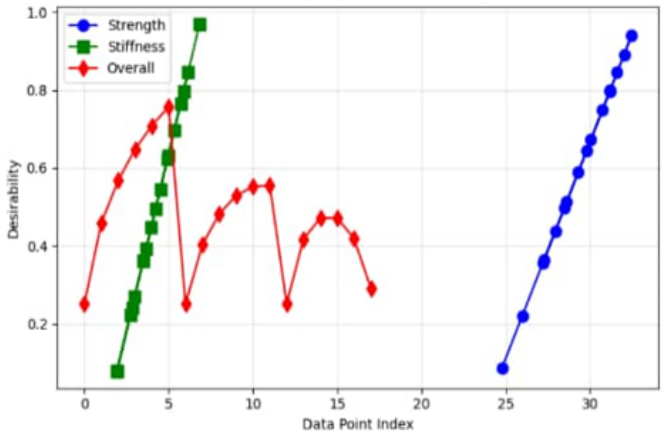


fig 14: contour plot of desirability (average over pksp wt.%)

Fig.12: The Consensus Analysis Results of Monte-Carlo Based Optimizations for The Experimental Result.



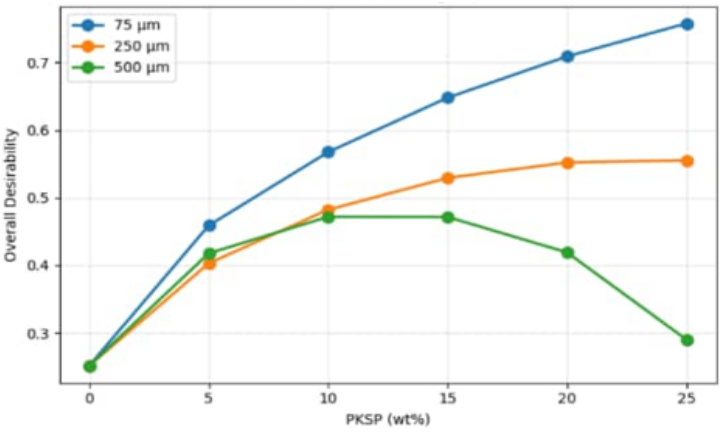
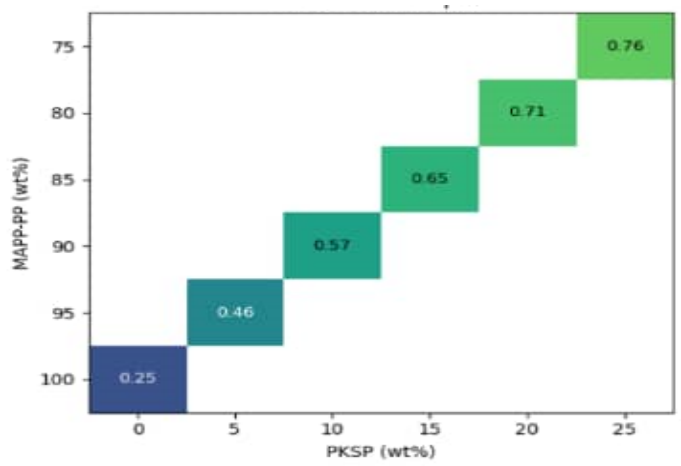


fig 15: individual and overall desirability

fig 16: pksp size x pksp wt.% interaction (mapp-pp average)



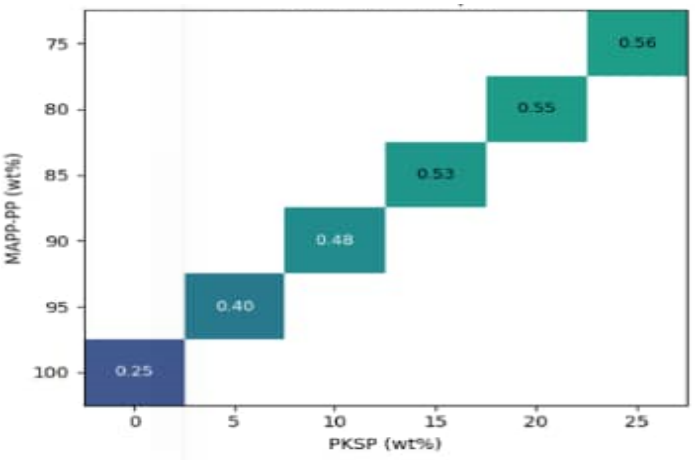


figure 17: desirability heatmap for 75µm pksp particle size

figure 18: desirability heatmap for 250µm pksp particle size

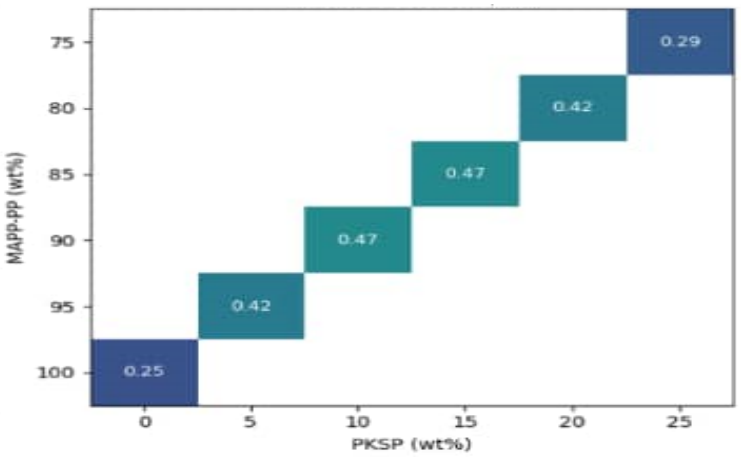


figure 19: desirability heatmap for 500µm pksp particle size

Key observations for the optimization results

Monte Carlo Optimization

Monte Carlo optimization conducted via a Python interface reveals that 25 wt% PKSP yields the highest weighted optimization scores across all particle sizes, with the 75 µm–25 wt% combination achieving the highest score. Pareto optimization similarly identifies 75 µm at 25 wt% as optimal, while product optimization shows that 25 wt% of either 75 µm or 500 µm maximizes the strength stiffness product. Geometric mean optimization ranks 75 µm at 25 wt% highest due to minimal variation in both properties across filler content. Desirability function analysis places 75 µm–25 wt% closely behind 500 µm–25 wt%. Consequently, the 75 µm–25 wt% combination emerges as the optimized set for achieving the best balance of strength and stiffness.

Based on these optimization results, the 75 µm–25 wt% formulation is considered highly suitable for applications requiring an optimal combination of strength and stiffness (with only marginal strength loss), when highly carbonized PKSP is used as a filler in compression-molded MAPP-reinforced PP/PKSP composites. The recommended expected material properties for this formulation are approximately 34.6 MPa and 4.82 GPa.

Alternative recommendations include the 500 µm–25 wt% formulation when maximum stiffness is prioritized, and the 75 µm–5 wt% formulation when maximum strength is the primary requirement, for the same filler requirement of highly carbonized PKSP.

IV. CONCLUSION

The experiment conducted via a Python interface reveals that 25 wt% PKSP yields the highest weighted optimization scores across all particle sizes, with the 75 µm–25 wt% combination achieving the highest score. Consequently, the 75 µm–25 wt% combination emerges as the optimized set for achieving the best balance of strength and stiffness, for the above-mentioned filler matrix This research confirms that MAPP-enhanced PP/PKSP composites, derived from agricultural waste, and highly optimized for strength-stiffness, presents a promising sustainable alternative for rigid food packaging applications, contributing to waste reduction and circular economy principles.

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