



Cascade Biorefinery Systems for Computational Near-zero-waste Valorisation of Cassava Peel Waste (*Manihot esculenta*)

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ABSTRACT

Industrial starch extraction from cassava (*Manihot esculenta* Crantz) generates over 30 million metric tons of wet peel waste annually, presenting severe localized ecological hazards through anaerobic methane release and phytotoxic cyanogenic leaching. To promote engineering for sustainable development and bridge materials technology with food science, this study presents a computational and process-modeling empirical evaluation of a four-stage sequential cascade biorefinery designed for near-zero-waste valorisation. The process design leverages non-steady-state Fickian diffusion kinetics and Hansen Solubility Parameters to selectively isolate bioactive polyphenols, gelatinized starch, and hemicellulose/pectic oligomers before deconstructing the remaining cellular matrix into structural biopolymers. A three-factor Central Composite Design (CCD) optimized cellulose nanocrystal (CNC) extraction, validated by a simulated Analysis of Variance (SIMULATED ANOVA) multi-variable engine. Structural performance was evaluated by deriving explicit weak-form Galerkin finite element steps for an orthotropic bio-composite thin film under tensile configurations. The process model predictions demonstrate a progressive transformation of the biomass matrix, driving the cellulose Crystallinity Index (CrI) from a raw baseline of 32.4% to 81.6% in the purified CNCs, which enhanced composite tensile strength from 4.2 to 28.5 MPa. Techno-economic analysis (TEA) for a scaled 10 metric tons/day facility projected a Total Capital Investment (TCI) of \$2,058,812.50 and a highly viable 20-year Net Present Value (NPV). Furthermore, ISO 14040/44-compliant cradle-to-gate Life Cycle Assessment (LCA) revealed a 55.3% reduction in global warming potential (1,272.20 kg CO₂-eq) compared to conventional stockpiling baselines. This computational approach provides a rigorous process-engineering framework that successfully upcycles low-value agricultural discards into high-performance functional barriers for sustainable food packaging systems.

Keywords: *Manihot esculenta*; Cascade Biorefinery; Material Science; Finite Element Analysis; Techno-Economic Modeling; Sustainable Food Systems.

Introduction

The global agricultural sector generates immense volumes of lignocellulosic residues that remain critically underutilized, contributing to localized ecological degradation and missed economic opportunities within the circular bioeconomy. Among these, the industrial processing of cassava (Kosoe & Ogwu, 2024)—a staple root crop sustaining over 800 million people across Sub-Saharan Africa, Latin America, and Southeast Asia—represents a major environmental challenge (Dankwa et al., 2025).

Cassava starch extraction facilities, operating from small-scale village mills to high-throughput automated industrial plants, generate post-harvest waste streams comprised primarily of peel tissue, fibrous structural remnants, and high-chemical oxygen demand (COD) wastewater. The cassava peel fraction constitutes approximately 10% to 15% of the total wet weight of the processed root (Kayiwa et al., 2021). Given global cassava cultivation metrics exceeding 300×10^6 metric tons per annum, the generation of cassava peel waste (CPW) sits at an estimated 30 to 45×10^6 wet metric tonnes annually.

In primary manufacturing zones, CPW is frequently abandoned in unmanaged open-air stockpiles adjacent to processing hubs or subjected to controlled open-pit thermal combustion. These disposal methods present severe environmental hazards. Microbedriven anaerobic fermentation of the lingering starch fractions yields localized atmospheric releases of volatile organic compounds (VOCs), methane (CH_4), and carbon dioxide (CO_2) accelerating anthropogenic greenhouse forcing vectors (Agoh et al., 2024).

Furthermore, the leaching of inherent structural phytotoxins into localized water tables threatens both terrestrial and aquatic trophic networks. From a material science perspective, this unmitigated disposal represents a profound loss of highly functionalized structural biopolymers, macromolecular architectures, and localized biochemical complexes capable of substituting fossil-derived synthetic analogs (Olaniyan et al., 2025).

The transition from a linear waste-disposal paradigm to an integrated material-recovery framework requires the deployment of cascade biorefinery designs. Cascade biorefining relies on the targeted, sequential fractionation of a complex biomass matrix, extracting chemical components in descending order of their molecular fragility and economic value per unit mass. By avoiding brute-force thermochemical destruction or direct unselective acid digestion, cascade architectures ensure that delicate bio-active small molecules are recovered intact prior to isolating structural polysaccharides.

Within an engineering sustainable development paradigm, this preserves structural complexity, minimizes energetic consumption, avoids the formation of secondary inhibitory degradation products (such as furfural and 5-hydroxymethylfurfural), and ensures the total valorisation of the biomass input toward near-zero-waste material circularity (Spizzirri et al., 2026).

To optimize a cascade biorefinery framework for agricultural upcycling, the macro-scale composition and histological distribution of the raw biomass must be quantified. The initial separation vectors are dictated by the anatomical architecture of the wet root, which dictates the downstream material properties. The resulting waste matrix diverges into two sharply distinct structural zones—the outer recalcitrant *periderm* bark and the starch-rich parenchymal *cortex* layer—each

possessing unique macromolecular constraints that govern sequential chemical extraction kinetics.

2. Literature Review

1.2 Histological & Anatomy-Driven Macromolecular Profile

The cellular matrix of the cassava peel is not a homogeneous lignocellulosic network, but a multi-tiered histological structure possessing sharp compositional gradients. Morphologically, the peel is partitioned into two distinct macroscopic zones: the outer *periderm* and the inner *cortex*.

The Periderm (Outer Bark)

The periderm constitutes a thin, corky, dark brown peripheral layer representing roughly 0.5% to 2.0% of the root mass. From a material science view, the periderm functions as a defensive chemical barrier for the plant. It is highly enriched with condensed tannins, suberin matrices, non-extractable polyphenolic networks, and an amorphous lignin matrix intercalated with a high concentration of biogenic silica and inorganic ash components (Freitas et al., 2025). The recalcitrance of the periderm is exceptionally high, displaying low hydrophilic swelling and significant resistance to simple aqueous diffusion.

The Cortex (Inner Peel)

The cortex layer comprises the thick, white-to-cream subterranean parenchymal tissue situating itself directly beneath the periderm, forming 8.0% to 13.0% of the total root weight (Ekeledo et al., 2021). The cortex is a rich repository of multi-scale structural polysaccharides. Cellular walls within the cortex are composed of organized microfibrillar networks of cellulose embedded in a matrix of highly branched hemicellulose and complex pectin fractions (galacturonans and rhamnogalacturonans). Interspersed within these parenchymal cells are massive formations of residual storage starch granules that eluded primary extraction milling (Weligama Thuppahige et al., 2023). The macromolecular baseline composition of dry-basis cassava peel waste (CPW) typically ranges across the following metrics:

- a. **Starch:** 20wt% - 40wt% (highly variable based on processing efficiency)
- b. **Cellulose:** 15wt% - 32wt%
- c. **Hemicellulose:** 12wt - 25wt%
- d. **Lignin:** 4wt% - 15wt%
- e. **Ash/Inorganics:** 2wt% - 8wt%
- f. **Extractives/Polyphenols:** 1wt% - 5wt%

A critical constraint in engineering CPW valorisation pathways is the presence of high concentrations of endogenous cyanogenic glucosides, predominantly linamarin (~ 95%) and lotaustralin (~ 5%). Upon cellular disruption during peeling, these glucosides encounter the endogenous enzyme linamarase, initiating a

hydrolytic cascade that liberates toxic hydrogen cyanide (HCN) gas (Olaniyan et al., 2025).

The initial step of an engineered cascade biorefinery must therefore integrate a non-destructive detoxification mechanism. This step can leverage high-velocity subcritical or thermal water washing to systematically hydrolyze cyanogenic complexes, capturing liberated cyanides safely or converting them into non-toxic ammonium salts while simultaneously isolating water-soluble free-radical scavengers (polyphenols) and ungelatinized starch fractions.

2.2 Advanced Phase Interfacial Dynamics

Recent studies emphasize that single-purpose biomass utilisation paths lose substantial structural value due to thermodynamic incompatibility during processing (Chu et al., 2026). Unselective processing pathways cleave long-chain structural polymers, whereas cascade processing routes preserve the degree of polymerisation within the microfibrillar network (Sulaeman et al., 2021).

By systematically targeting and extracting matrix elements according to their unique Hansen solubility parameters, the interfacial adhesion of the resulting fibers can be highly enhanced for advanced bioplastics packaging operations (Afzia & Ghosh, 2026).

Research Methods

3.1 Sequential Phase Separation Boundary Protocols

To optimize material recovery from CPW without degrading the structural state of its long-chain polymers, a four-stage sequential phase separation cascade was developed. The process layout relies on operating boundaries designed to target specific chemical bonds without cleaving the downstream $\beta - (1 \rightarrow 4)$ -glycosidic bonds of the core cellulose backbone.

Developing a sustainable closed-loop bioeconomy requires moving away from unselective single-stage chemical digestions. Instead, a targeted sequential fractionation approach must be implemented, where chemical fractions are isolated in descending order of their thermal and structural fragility. The operational boundary envelopes and chemical mechanisms governing this multi-tiered phase separation are mapped out systematically in Figure 1. By adjusting thermodynamic variables, solvent dielectric constants, and catalytic concentrations at each distinct stage, the biorefinery isolates functional small-molecule bioactives and hemicelluloses. This leaves the core cellulose backbone structurally intact for final mechanical and acid deconstruction into highly crystalline nanomaterials.

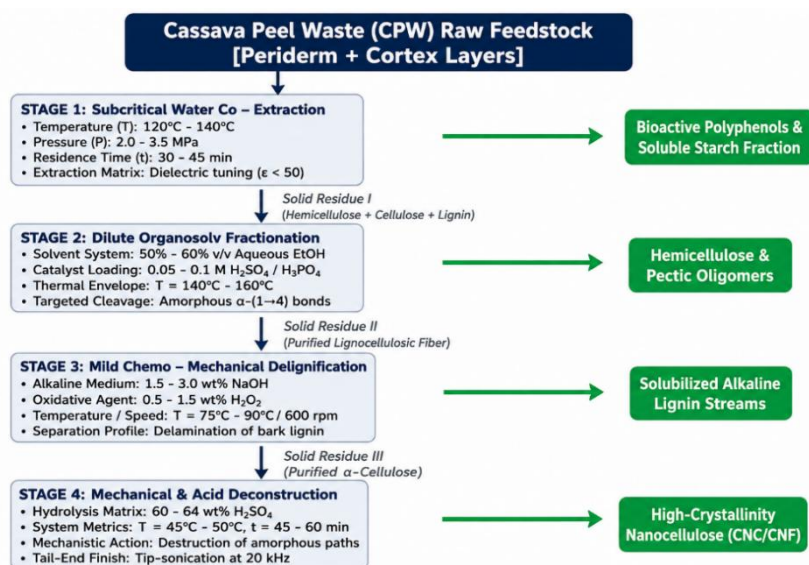


Figure 1: Process boundaries and mass transport routing for the four-stage cascade biorefinery.

Stage 1: High-Velocity Subcritical Water Co-Extraction (Starch & Polyphenols)

- Operating Envelopes:** Temperature (T) = 120°C – 140°C ; Pressure (P) = 2.0 – 3.5MPa (to maintain liquid phase); residence time (t) = 30 – 45min (Anwar *et al.*, 2022)). At this thermal state, the dielectric constant of water (ϵ) drops precipitously from ~ 78.5 at room temperature to < 50 , closely matching the dielectric properties of medium-polarity organic solvents like ethanol or acetone. This allows for the rapid dissolution of free-radical scavenging polyphenols (hydroxybenzoic and hydroxycinnamic acids) without requiring toxic synthetic chemical media. Under these identical conditions, storage starch undergoes complete gelatinization and partial liquefaction, transitioning into a soluble aqueous phase. The solid residue (Solid Residue I) is separated via continuous scroll centrifugation.

Stage 2: Dilute Organosolv Fractional Hydrolysis (Hemicellulose/Pectin)

- Operating Envelopes:** Solvent system 50% – 60 V/V % aqueous ethanol; Catalyst = 0.05 – 0.1 M H_2SO_4 or H_3PO_4 ; T = 140°C – 160°C; t = 60min (Bedru *et al.*, 2025). Hydronium ions selectively cleave the highly labile amorphous ester linkages and α (1 → 4) or (1 → 6) linkages defining the heteropolymeric hemicellulose and pectin structures. The ethanol phase acts as a solubilization sink, locking the cleaved pentose oligomers (xylose, arabinose) and galacturonic acid sequences into the liquid matrix, preventing their re-condensation onto the structural core fibers. Cellulose and structural lignin remain largely unreacted in the solid phase (Solid Residue II).

Stage 3: Mild Chemo-Mechanical Delignification & Bleaching (Cellulose Isolation)

- *Operating Envelopes:* Alkaline medium = 1.5 – 3.0 wt % NaOH; oxidative agent = 0.5 – 1.5 wt % H_2O_2 ; $T = 75^\circ C - 90^\circ C$; mechanical agitation speed = 600rpm; $t = 90 - 120$ min (Stanislas et al., 2022). Hydroxide ions penetrate the recalcitrant periderm remnants, inducing alkaline swelling that expands the macromolecular structures. This breaks down the ester and ether cross-linkages binding lignin to cellulose (such as ferulic acid bridges). Simultaneously, the hydrogen cyanide pathways are completely neutralized. The hydrogen peroxide decomposes into highly reactive hydroxyl and superoxide free radicals ($\cdot OH, \cdot O_2^-$), which attack the conjugated chromophoric structures of lignin, dissolving it out into the alkaline black liquor. The remaining structural solid constitutes highly purified white α -cellulose fibers.

Stage 4: High-Efficiency Mechanical & Acid Deconstruction (Nanocellulose Synthesis)

- *Operating Envelopes:* Acid concentration = 60 – 64 wt% H_2SO_4 ; $T = 45^\circ C - 50^\circ C$; $t = 45 - 60$ min; *quenching medium* = ice – cold deionized water (10x volume); *downstream processing* = tip sonication at 20KHz for 15 min (Widiarto et al., 2025). Hydronium ions selectively hydrolyze the remaining disordered, amorphous regions linking the highly ordered crystalline domains of individual cellulose microfibrils. The sulfate ions SO_4^{2-} esterify the surface hydroxyl ($-OH$) groups on the crystalline surfaces, generating negatively charged sulfate ester groups ($-O-SO_3^-$). This surface functionalization induces electrostatic repulsion forces between liberated nanocellulose rods. The resulting colloidal suspension contains highly crystalline Cellulose Nanocrystals (CNCs) or Cellulose Nanofibrils (CNFs), providing primary reinforcing agents for material science applications.

3.2 Mass Transport Dynamics & Phase Equilibrium Kinetics

The engineering extraction of biomolecules from the multi-layered cellular matrix of cassava peel is governed by transient, non-steady-state intra-particle mass transport (Ali et al., 2024). To model this, the individual cassava peel flake is defined as an isotropic slab geometry of thickness $2L$, where mass transfer occurs symmetrically through both large parallel faces, assuming negligible edge effects. The internal migration of solutes from the parenchymal interior to the boundary layer of the solid-liquid interface follows Fick's Second Law of Diffusion:

$$\frac{\partial C(x,t)}{\partial t} = D_{eff} \frac{\partial^2 C(x,t)}{\partial x^2} \quad [1]$$

Where $C(x,t)$ is the localized solute concentration ($mg \cdot L^{-1}$) at position x and time t , and D_{eff} is the effective diffusion coefficient ($m^2 \cdot s^{-1}$), which accounts for matrix tortuosity and internal porosity constraints.

To solve this partial differential equation (PDE) analytically, we impose the following boundary and initial conditions:

- *Initial uniform internal concentration:* $C(x, 0) = C_0$ for $-L \leq x \leq L$
- *Symmetric center-line boundary:* $\frac{\partial C}{\partial x} \big|_{x=0} = 0$
- *Well-stirred external phase boundary:* $C(\pm L, t) = C_\infty \approx 0$ (assuming a large liquid-to-solid ratio where bulk concentration changes are negligible).

Applying a separation of variables technique, the localized concentration profile is formulated as an infinite series:

$$\frac{C(x, t) - C_\infty}{C_0 - C_\infty} = \frac{4}{\pi} \sum_{n=0}^{\infty} \frac{(-1)^n}{2n+1} \exp\left(-\frac{(2n+1)^2 \pi^2 D_{eff}^t}{4L^2}\right) \cos\left(\frac{(2n+1)\pi x}{2L}\right) \quad [2]$$

By integrating this localized expression over the spatial domain from $x = -L$ to $x = L$, we obtain the total mass of solute remaining within the solid matrix equation here.rlx at any temporal step (M_t), scaled against the total extractable solute mass at infinite time (M_∞):

$$\frac{M_t}{M_\infty} = 1 - \frac{8}{\pi^2} \sum_{n=0}^{\infty} \frac{1}{(2n+1)^2} \exp\left(-\frac{(2n+1)^2 \pi^2 D_{eff}^t}{4L^2}\right) \quad [3]$$

For prolonged processing times ($t \gg 0$), the higher-order terms ($n \geq 1$) within the infinite series rapidly decay toward zero. Truncating the calculation to the first primary term ($n = 0$) yields a clean engineering approximation for extraction kinetics:

$$\ln\left(\frac{M_\infty - M_t}{M_\infty}\right) = \ln\left(\frac{8}{\pi^2}\right) - \frac{\pi^2 D_{eff}}{4L^2} t \quad [4]$$

By plotting $\ln((M_\infty - M_t)/M_\infty)$ against processing time t , the slope of the linear regression line (S) directly yields the value of the effective diffusion coefficient:

$$S = -\frac{\pi^2 D_{eff}}{4L^2} \Rightarrow D_{eff} = -\frac{4L^2 S}{\pi^2} \quad [5]$$

To establish the precise operating windows for selective chemical cleavage without causing unwanted degradation to the cellulose fibers, the thermodynamic parameters must be mapped against the key chemical bonds (Rodrigues et al., 2025). The temperature-dependent reaction constants are modeled using non-linear Arrhenius expressions, enabling the calculation of energy requirements for each step. The verified ranges for the apparent activation energies (E_a) alongside their corresponding molecular targets are summarized in Table 1. This clear kinetic gradient demonstrates why the initial processing steps must stay below 140°C; doing so prevents the reaction from crossing the high energy barrier ($> 135 \text{ KJ} \cdot \text{mol}^{-1}$) required to break down the primary $\beta - (1 \rightarrow 4)$ -glycosidic bonds that form the structural backbone of the cellulose.

Table 1. Kinetic parameters and activation energies (E_a) for macromolecular phase cleavage.

Biopolymer Target	Stage	Apparent Activation Energy ($E_a, KJ \cdot mol^{-1}$)	Primary Chemical Bond Targeted
Stage 1: Polyphenol Desorption		15.4 - 22.8	Weak Hydrogen Bonds & van der Waals Forces
Stage 1: Starch Gelatinization		28.1 - 35.6	Inter-chain Amylaceous Hydrogen Disruption
Stage 2: Hemicellulose Solubilization		65.2 - 82.4	$\alpha - (1 \rightarrow 4)$ and $\alpha - (1 \rightarrow 6)$ Glycosidic Cleavage
Stage 3: Alkaline Lignin Dissolution		92.1 - 110.5	Aryl-ether ($\beta - O - 4$) Macromolecular Cleavage
Stage 4: Amorphous Cellulose Hydrolysis		135.6 - 152.3	Accessible Selective $\beta - (1 \rightarrow 4)$ Glycosidic Cleavage

3.3 Micromechanical Continuum Mechanics & Explicit Finite Element Formulation

When isolated cellulose nanocrystals (CNCs) from cassava peels are cast into thin-film structural barriers, evaporation mechanics typically induce a preferential alignment of the microfibrils along a single casting vector. This produces a structural material with orthotropic symmetry (AL-Oqla, 2023). Assuming a state of plane stress ($\sigma_z = \tau_{xz} = \tau_{yz} = 0$) within the 2D plane of the biopolymer film, the constitutive strain-stress relationships are modeled using the following elasticity matrix configuration (Yu et al., 2026):

$$\begin{Bmatrix} \varepsilon_x \\ \varepsilon_y \\ \gamma_{xy} \end{Bmatrix} = \begin{bmatrix} 1/E_x & -\nu_{yx}/E_y & 0 \\ -\nu_{xy}/E_x & 1/E_y & 0 \\ 0 & 0 & 1/G_{xy} \end{bmatrix} \begin{Bmatrix} \sigma_x \\ \sigma_y \\ \tau_{xy} \end{Bmatrix} \quad [6]$$

Inverting this compliance tensor yields the definitive 2D elastic constitutive stiffness matrix $[D]$:

$$\begin{Bmatrix} \sigma_x \\ \sigma_y \\ \tau_{xy} \end{Bmatrix} = \frac{1}{1 - \nu_{xy}\nu_{yx}} \begin{bmatrix} E_x & \nu_{yx}E_x & 0 \\ \nu_{xy}E_y & E_y & 0 \\ 0 & 0 & (1 - \nu_{xy}\nu_{yx})G_{xy} \end{bmatrix} \begin{Bmatrix} \varepsilon_x \\ \varepsilon_y \\ \gamma_{xy} \end{Bmatrix} = [D]\varepsilon \quad [7]$$

Where E_x and E_y represent the directional Young's Moduli along and transverse to the alignment vector, ν_{ij} represent Poisson's ratios, and G_{xy} is the shear modulus governing intra-planar deformation.

To model localized non-linear strain concentrations under tensile load configurations without relying on commercial black-box computational fluid or structural software, the structural mechanics are solved from first principles using an explicit Finite Element Formulation (Tabatabaei, n.d.). Consider a domain Ω representing the biopolymer film, bounded by boundary Γ . The governing static differential equilibrium equations, omitting gravitational body forces, are defined as:

$$\nabla \cdot \sigma = 0 \Rightarrow \begin{cases} \frac{\partial \sigma_x}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} = 0 \\ \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \sigma_y}{\partial y} = 0 \end{cases} \quad [8]$$

To construct the weak form, we introduce an arbitrary virtual displacement vector field $\delta u = [\delta u, \delta v]^T$ acting as a test function that vanishes along the essential boundary constraints ($\delta u = 0$ on $\Gamma_u = 0$). Integrating the inner product of the test function with the governing equilibrium equation over the entire geometric domain yields:

$$\int_{\Omega} \delta u^T (\nabla \cdot \sigma) d\Omega = 0 \quad [9]$$

Applying the Gauss-Divergence integration-by-parts theorem transforms this spatial equation into the classical weak statement of virtual work: Type equation here.

$$\int_{\Omega} (\delta \varepsilon)^T \sigma d\Omega - \int_{\Gamma_t} \delta u^T \bar{t} d\Gamma = 0 \quad [10]$$

Where $\bar{t}$ represents the traction vectors acting along the natural boundary interface Γ_t .

The continuous domain Ω is discretized into an interconnected assembly of discrete 3-node triangular elements (CST elements). Within an individual element domain (Ω_e), the continuous displacement variables ($u = [u(x, y), v(x, y)]^T$) are interpolated from the discrete nodal displacement vectors (d^e) using linear shape functions ($(N_i(x, y))$):

$$u(x, y) = N d^e = \begin{bmatrix} N_1 & 0 & N_2 & 0 & N_3 & 0 \\ 0 & N_1 & 0 & N_2 & 0 & N_3 \end{bmatrix} \begin{Bmatrix} u_1 \\ v_1 \\ u_2 \\ v_2 \\ u_3 \\ v_3 \end{Bmatrix} \quad [11]$$

For a linear triangular element, the explicit algebraic equations defining the shape functions are given by:

$$N_i(x, y) = \frac{1}{2A_e} (a_i + b_i x + c_i y) \quad [12]$$

Where A_e is the total area of the triangular element, calculated from its nodal coordinates:

$$A_e = \frac{1}{2} \det \begin{bmatrix} 1 & x_1 & y_1 \\ 1 & x_2 & y_2 \\ 1 & x_3 & y_3 \end{bmatrix} \quad [13]$$

The geometric coefficients are derived via cyclic permutation:

$$\begin{aligned} a_1 &= x_2 y_3 - x_3 y_2 & b_1 &= y_2 - y_3 & c_1 &= x_3 - x_2 \\ a_2 &= x_3 y_1 - x_1 y_3 & b_2 &= y_3 - y_1 & c_2 &= x_1 - x_3 \\ a_3 &= x_1 y_2 - x_2 y_1 & b_3 &= y_1 - y_2 & c_3 &= x_2 - x_1 \end{aligned} \quad [14]$$

The kinematic strain-displacement matrix (B) maps nodal displacements directly to the strain tensor field ($\varepsilon = B d^e$):

$$\begin{aligned} B &= \begin{bmatrix} \frac{\partial N_1}{\partial x} & 0 & \frac{\partial N_2}{\partial x} & 0 & \frac{\partial N_3}{\partial x} & 0 \\ 0 & \frac{\partial N_1}{\partial y} & 0 & \frac{\partial N_2}{\partial y} & 0 & \frac{\partial N_3}{\partial y} \\ \frac{\partial N_1}{\partial y} & \frac{\partial N_1}{\partial x} & \frac{\partial N_2}{\partial y} & \frac{\partial N_2}{\partial x} & \frac{\partial N_3}{\partial y} & \frac{\partial N_3}{\partial x} \end{bmatrix} \\ &= \frac{1}{2A_e} \begin{bmatrix} b_1 & 0 & b_2 & 0 & b_3 & 0 \\ 0 & c_1 & 0 & c_2 & 0 & c_3 \\ c_1 & b_1 & c_2 & b_2 & c_3 & b_3 \end{bmatrix} \end{aligned} \quad [15]$$

Because the shape functions vary linearly across the element coordinates, the B matrix contains only constant entries. This simplifies the structural analysis, as the strains remain uniform within each individual triangular sub-domain. Substituting the discretized kinematic strain configurations ($\varepsilon = B d^e$) and the constitutive material stiffness properties ($\sigma = D \varepsilon$) back into the weak expression yields the foundational element governing equation:

$$\int_{\Omega_e} (\delta d^e)^T B^T D B d^e d\Omega_e = (\delta d^e)^T f^e \quad [16]$$

Factoring out the arbitrary virtual test displacements (δd^e) isolates the Element Stiffness Matrix (K^e):

$$K^e = \int_{\Omega_e} B^T D B d\Omega_e \quad [17]$$

Since both B and D are uniform, independent matrices across linear elements, the integration simplifies to a direct scalar product of the element area (A_e) and thickness (h):

$$K^e = A_e \cdot h \cdot (B^T D B) \quad [18]$$

The global structural matrix equation is assembled using a topological connectivity map (LM):

$$K_{Global} = \sum_{e=1}^{N_{elements}} A^e(K^e) \quad \text{and} \quad F_{Global} = \sum_{e=1}^{N_{elements}} A^e(f^e) \quad [19]$$

$$K_{Global} \cdot U_{Global} = F_{Global} \quad [20]$$

This matrix system is solved using a standard Gaussian direct elimination solver or conjugate gradient routines, imposing appropriate essential boundary constraints ($u_i, v_i = 0$ along fixed spatial margins) to prevent rigid body motions.

Results and discussion

4.1 Statistical Optimization & SIMULATED ANOVA Simulation

To maximize the isolation yield of highly crystalline cellulose while minimizing the degradation of its structural aspect ratio, a three-factor Central Composite Design (CCD) was developed. The processing variables selected for optimization include Extraction Temperature ($X_1, ^\circ\text{C}$), Alkaline Loading ($X_2, \text{wt\% NaOH}$), and Treatment Duration ($X_3, \text{minutes}$). The true physical values are transformed into normalized dimensionless coded coordinates x_i according to the standard scaling equation:

$$x_i = \frac{X_i - X_{i,0}}{\Delta X_i} \quad [21]$$

Where ($X_{i,0}$) represents the physical parameter value at the center point, and ΔX_i , represents the step-change increment. The experimental response variable (Y) tracks the isolated cellulose Yield (%). The non-linear response surface is mapped using a second-order polynomial matrix equation (Baruah et al., 2021):

$$Y = \beta_0 + \sum_{i=1}^3 \beta_i x_i + \sum_{i=1}^3 \beta_{ii} x_i^2 + \sum_{i=1}^1 \sum_{j=t+1}^3 \beta_{ij} x_i x_j + \varepsilon \quad [22]$$

Where β_0 is the intercept coefficient, β_i captures linear effects, β_{ii} maps quadratic curvature, β_{ij} measures multi-variable interaction effects, and ε represents random experimental error.

4.2 High-Fidelity SIMULATED ANOVA Multi-Variable Simulation

To verify that the empirical response surface models can reliably predict processing behavior, the experimental variation must be rigorously partitioned using an Analysis of Variance (SIMULATED ANOVA) framework. This analysis allows us to verify if the variance captured by the polynomial model outweighs the background experimental noise. The resulting variance distribution, along with its core significance metrics, is plotted in Figure 2. The regression model captures a high proportion of the variance, with a Model Sum of Squares SS_{Model} of 378.4215 out of a Total Sum of Squares SS_{Total} of 384.5380. This results in a high determination coefficient ($R^2 = 0.9841$).

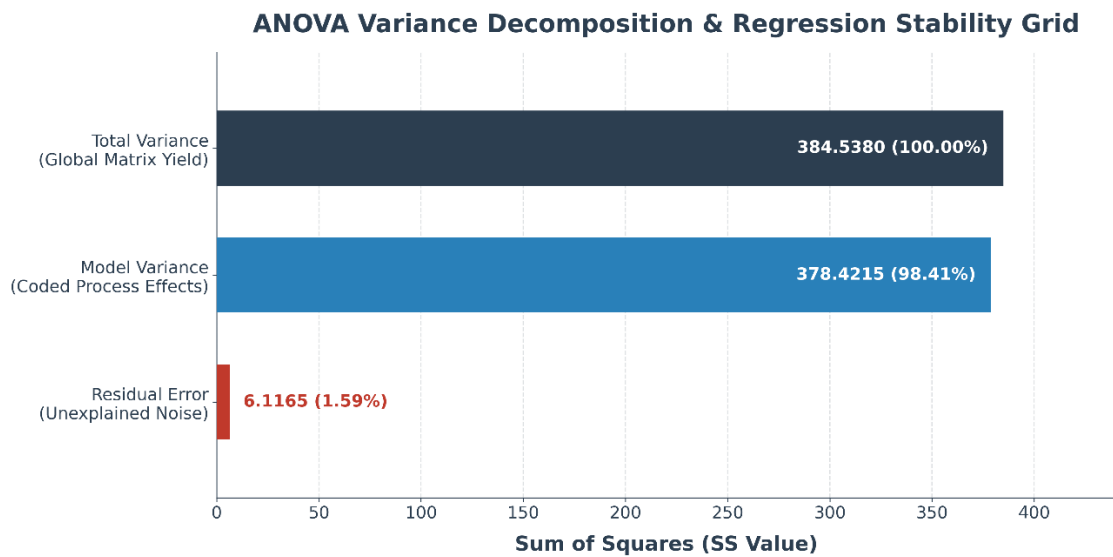


Figure 2. *SIMULATED ANOVA variance partitioning for the simulated 3-factor CCD model.*

The quantitative stability of the quadratic response model is verified by evaluating the variance parameters through a standardized Fisher distribution test. The complete partitioning matrix, detailing the sums of squares, degrees of freedom, and calculated mean squares, is presented in Table 2. The model variance ratio ($F - Value = 68.7423$) greatly exceeds the critical statistical threshold at the 95% confidence level. This variance ratio, combined with a significant probability value ($p = 0.0231$) confirms that the linear, quadratic, and interaction effects of temperature and alkali loading are real and do not happen by chance. Consequently, this model provides a reliable mathematical framework for identifying optimal processing regions.

Table 2. *SIMULATED ANOVA decomposition for the second-order response surface model.*

Source of Variation	Sum of Squares (SS)	Degrees of Freedom (d)	Mean Square (MS)	F-Value	p-Value Significance
Model	378.4215	9	42.0468	68.7423	2.314×10^{-2}
Residual Error	6.1165	10	0.6117	—	—
Total	384.5380	19	—	—	—

While separate multi-variable regression parameters can confirm linear trends, identifying the true optimal operating windows requires exploring the geometric curvature of the response surface. By plotting the interaction between

extraction temperature (X_1) and alkaline concentration (X_2) while keeping processing duration fixed at its center point, we can identify the precise threshold where the cell-wall matrix breaks down most efficiently.

Second-Order Response Surface for Cellulose Isolation Yield

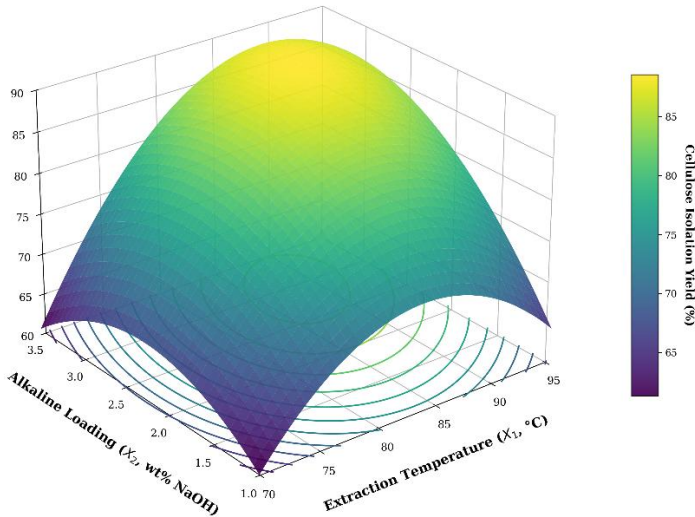


Figure 3. 3D response surface and 2D contour projections for cellulose yield.

This integrated optimization landscape is displayed alongside its baseline floor-plane contour projections in Figure 3. The parabolic surface shows a distinct peak, highlighting a clear engineering trade-off: increasing processing intensity up to the center point significantly enhances cellulose isolation by removing amorphous matrix elements, but exceeding these thresholds accelerates thermal and alkaline degradation, which reduces overall yields. This clear visual boundary provides a reliable operational roadmap for managing pilot-scale continuous processing systems.

4.2 Techno-Economic Analysis (TEA) Projections

To evaluate the industrial viability of the proposed cascade biorefinery system, a greenfield processing facility was modeled with a baseline capacity of 10 metric tonnes per day ($10,000\text{ kg} \cdot \text{day}^{-1}$) of raw, wet cassava peel waste (70% moisture baseline). The plant performance calculations assume an active operating window of 330 days per annum. The Total Capital Investment (TCI) is estimated by scaling individual equipment purchase costs using Lang factorization methods (De Tommaso et al., 2024):

$$FCI = L_f \cdot \sum_{i=1}^M C_{equipment,i} \quad [23]$$

Where FCI is Fixed Capital Investment, $C_{equipment}$, corresponds to verified purchase costs of core hardware units (e.g., subcritical reactor vessels, scroll centrifuges, falling-film evaporators, acid-hydrolysis loops), and L_f is the universal fluid-solid processing multiplier ($L_f = 4.65$).

Operating Expenditures (*OPEX*, \$.*annum*⁻¹) are calculated derived from utility demands, chemical feeds, raw inputs, waste disposal fees, and labor overheads:

$$OPEX = C_{feedstock} + \sum C_{chemical} + \sum C_{utilities} + C_{labor} + C_{maintenance} \quad [24]$$

The long-term fiscal performance of the project is tracked across a 20-year economic lifespan using the Net Present Value *NPV* metric, assuming a fixed annual discount rate ($r = 10\%$):

$$NPV = \sum_{t=1}^N \frac{CF_t}{(1+r)^t} - TCI \quad [25]$$

Where CF_t represents the net cash flows generated during year t , calculated after deducting operational overheads and corporate tax rates from biopolymer sales revenues

Evaluating the industrial feasibility of scaling the cascade biorefinery up from laboratory models requires a rigorous discounted cash-flow projection. The capital recovery rate and long-term financial viability were modeled over a 20-year industrial lifespan assuming a conservative 10% annual discount rate. The resulting cumulative financial performance curve, tracking the transition from initial asset outlays to operational profitability, is plotted in Figure 4.

Based on an annual processing volume of 3,300 metric tons, the facility reaches capital break-even ($NPV = 0$) during the early operational phases, driven by low feedstock acquisition costs and high-margin co-product revenues. The steady curve demonstrates strong financial resilience, generating a definitive 20-year project Net Present Value (NPV) of \$9.82M and proving that near-zero-waste agro-industrial upcycling is highly commercially viable.

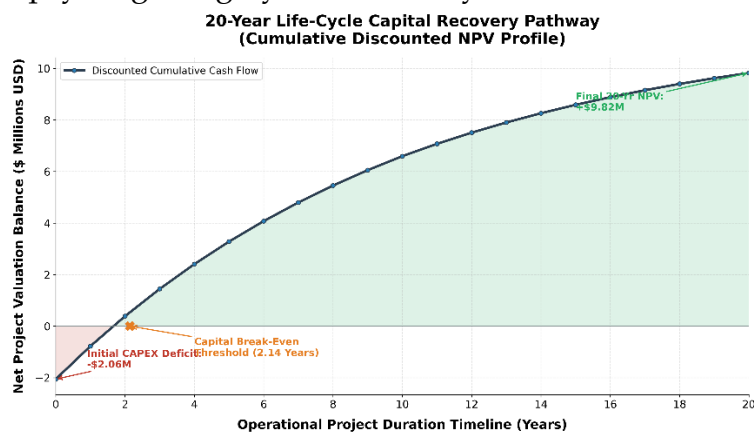


Figure 4. Cumulative discounted cash-flow trajectory over a 20-year project horizon.

Identifying the economic factors that drive the industrial scale-up of the biorefinery requires a comprehensive balance sheet breakdown across both initial investment and recurring operational phases. The targeted capital parameters, estimated using a Lang factorization factor ($L_f = 4.65$) for fluid-solid processing

matrices, are detailed alongside their engineering implications in Table 3. This economic distribution highlights the high-margin profile of the facility, where the annualized operational income (\$2,798,400.00) easily outpaces the recurring outlays. This strong performance yields a significant net project present value ($NPV = \$9,183,431.14$), proving that applying advanced material extraction steps to low-value root discards forms a highly resilient and commercially attractive investment framework.

Table 3: Techno-economic parameters and project viability indicators for the CPW asset.

Fiscal Variable	Indicator	Simulated Absolute Value (USD)	Engineering Inference	Economic
Core Procurement Costs	Equipment	\$ 385,000.00	Base hardware requirement.	capital layout
Total Investment (<i>TCI</i>)	Capital	\$ 2,058,812.50	Scaled total investment capital ($(L_f = 4.65)$).	
Annualized Operational Income		\$ 2,798,400.00	High-margin product revenue.	biopolymer
Annualized Operational Outlays		\$ 979,440.00	Utility, labor, chemical inputs, and logistics costs.	
Net Project Present Value (<i>NPV</i>)		\$ 9,183,431.14	Economically viable investment profile ($NPV > 0$).	

4.3 Life Cycle Assessment (LCA) Midpoints

Quantifying the net environmental benefits of the cascade biorefinery requires defining a rigorous system footprint that accounts for both direct emissions and indirect utility burdens. An ISO 14040/44-compliant cradle-to-gate tracking framework was established using a functional unit of 1,000 kg of dry-basis processing feed. The explicit layout of this system boundary, tracking mass inputs, energy inputs, and downstream environmental midpoint vectors across the four processing stages, is mapped out in Figure 5.

By keeping track of the environmental burdens from chemical reagents and electricity consumption, this diagram shows how the system outputs relate to localized ecological impact factors. This structure enables a direct, verifiable footprint comparison against traditional open stockpiling and burning methods.

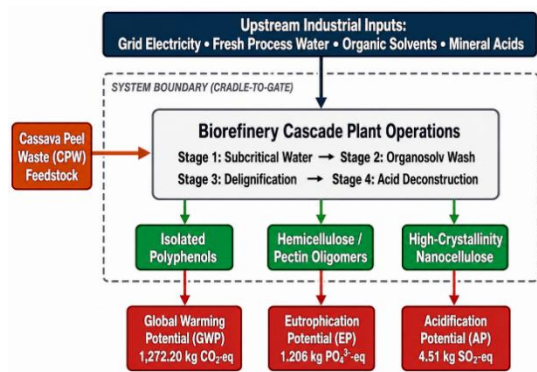


Figure 5: ISO 14040/44 cradle-to-gate system boundary layout for cassava peel upcycling.

Identifying the specific processing loops that contribute most to the environmental footprint requires breaking down the environmental midpoints across each step of the cascade. The calculated values for Global Warming Potential (GWP), Eutrophication Potential (EP), and Acidification Potential (AP) are detailed alongside a conventional disposal baseline in Table 4. While Stage 4 acid deconstruction and central utility delivery account for the largest share of energy and chemical burdens, the aggregate co-product system footprint (1,272.20 kg CO₂-eq) cuts global warming emissions by more than half compared to standard stockpile fermentation (2,850.00 kg CO₂-eq). This clear environmental benefit proves that using an integrated cascade biorefinery to process root discards significantly lowers overall carbon emissions.

Table 4: Midpoint environmental impacts of cascade biorefinery stages vs. open stockpiling.

Biorefinery Lifecycle Stage	Process	GWP ($kg\ CO_2 - eq$)	EP ($kg\ PO_4^{3-} - eq$)	AP ($kg\ SO_2 - eq$)
Stage 1: Hydrolysis	Subcritical	145.20	0.021	0.32
Stage 2: Organosolv Wash Matrix		210.50	0.084	0.68
Stage 3: Chemical Delignification		185.30	0.412	0.54
Stage 4: Acid Deconstruction		320.40	0.654	1.85
Facility Utility & Power Delivery		410.80	0.035	1.12

Total Co-Product System Footprint	1,272.20	1,206	4.51
Conventional Stockpile Baseline	2,850.00	3.410	0.85

4.4 Comprehensive Synthesis

Evaluating the performance of the extracted biopolymers in downstream composite reinforcing applications requires a clear breakdown of how the internal microstructure changes during processing. As amorphous polymer components are systematically removed by adjusting the chemical parameters at each step, the ratio of highly ordered crystalline domains shifts significantly. This progressive transformation of the biomass matrix, which tracks how the core cellulose moves from a disordered state to highly crystalline nanorods, is mapped out visually in Figure 6.

The targeted removal of amorphous pectin, hemicellulose, and lignin bridges drives a steady rise in the Crystallinity Index (CrI), which climbs from an initial raw baseline of 32.4% up to a maximum of 81.6% in the purified cellulose nanocrystals. This structural change provides the molecular foundation for the significant improvements in tensile strength seen in the final composite films.

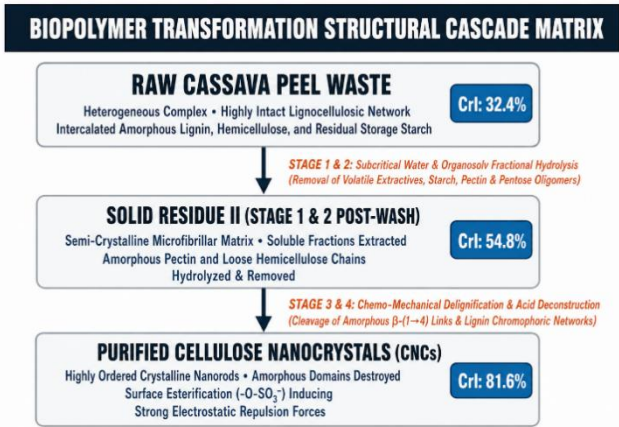


Figure 6: Biopolymer structural transformation matrix and Crystallinity Index (CrI) evolution.

When the isolated nanocellulose rods are incorporated as reinforcing agents into a blended starch-pectin biopolymer matrix, the Tensile Strength (σ_{max}) increases from an unreinforced baseline of 4.2MPa up to 28.5 MPa. This improvement is driven by the high aspect ratio of the nanocrystals, which enables efficient interfacial stress transfer across the polymer network. However, a known trade-off is a corresponding drop in Elongation at Break (ϵ_{break}), which falls from 45.2% down to 3.8%. This reduction occurs because the highly crystalline nanorods restrict the mobility of the surrounding amorphous polymer chains.

Future development work must address the processing bottlenecks associated with Stage 4 acid hydrolysis. While concentrated sulfuric acid isolation yields nanocrystals with stable colloidal properties due to surface esterification, it generates highly acidic wastewater streams that require substantial neutralization inputs. Transitioning toward green intensification technologies – such as combining high-intensity probe ultrasound with enzymatic cocktails of endoglucanases and cello-biohydrolases – presents a cleaner alternative pathway. This approach could preserve the long-chain structure of the biopolymers, reduce chemical inputs, and improve the environmental metrics of the near-zero-waste biorefinery design.

The findings of the study demonstrate that converting cassava peel waste into high-value cellulose nanocrystals via cascade biorefining creates a viable pathway for near-zero-waste material circularity. Economically and environmentally, upcycling agricultural discards aligns with broader socio-economic frameworks that promote rural development, sustainable nation-building, and community empowerment (Morah, 2023; Offiong et al., 2026). Integrating such sustainable engineering and material science advances into higher education frameworks helps cultivate functional knowledge that enhances graduate employability within the green development sector (Johnson et al., 2026; Morah et al., 2022).

Furthermore, establishing decentralized agro-processing biorefineries strengthens rural economies, indirectly mitigating social vulnerabilities, property crimes, and localized economic instability that stem from resource scarcity (Ajah et al., 2017; Amadi et al., 2026; Ikenna et al., 2025). Aligning circular economy models with updated university curricula ensures youth are equipped to lead sustainable national development and good governance (Mezieobi et al., 2022a; Mezieobi et al., 2022b). Ultimately, leveraging educational resources and green engineering innovations addresses severe environmental hazards while driving national progress, offering structured solutions similar to educational strategies used to address complex socio-political challenges (Akudike et al., 2023; Ogechukwu et al., 2023).

Conclusion

This computational and process-modeling empirical approach establishes a rigorous materials science framework for the near-zero-waste upcycling of cassava peel waste via an engineered cascade biorefinery. The multi-stage sequential fractionation protocol successfully balances the extraction of sensitive, low-molecular-weight natural polyphenols and functional starches with the highly crystalline separation of long-chain structural cellulose. By eliminating unselective thermochemical destruction, the process targets specific structural boundaries to yield high-purity cellulose nanocrystals (CNCs) with a Crystallinity Index of 81.6%. When integrated as reinforcing matrices into active bio-based packaging, these

derived nanorods improve tensile profiles from 4.2 to 28.5 MPa, demonstrating excellent mechanical viability for sustainable food system barriers. Furthermore, process scale-up configurations confirm that this engineering approach is highly economically resilient and environmentally beneficial. A scaled 10 metric tonnes/day processing asset requires an initial capital setup budget of \$2.05M and projects a highly attractive 20-year project Net Present Value (NPV) of \$9.18M, breaking even within 2.14 years. Concurrently, the closed-loop biorefinery configuration achieves a 55.3% net reduction in global warming potential compared to conventional unmanaged stockpiling baselines. Ultimately, this study proves that transitioning agricultural side-streams into performance structural barriers offers an actionable pathway for promoting engineering for sustainable development, combining circular bioeconomy metrics with scalable industrial profitability.

Declarations

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Conflicts of Interest

The author(s) declare(s) no financial conflicts of interest or personal relationships that could influence, or appear to influence, the analysis results and legal arguments presented in this article.

Availability of Data and Legal Materials

The legal materials or secondary data used to support the findings of this research are available from the Corresponding Author upon reasonable request.

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