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Review

AI-Assisted Business Strategies and Markets for Products Derived from Agri-Food Waste and By-Products

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Abstract: Agri-food waste valorisation is constrained by feedstock heterogeneity, process uncertainty, volatile markets, and evolving regulation, which collectively increase business risk and delay market entry. This review synthesizes evidence on how artificial intelligence (AI) reduces these uncertainties and enables opportunity identification and decision support across the valorisation value chain. At intake, AI coupled with rapid sensing supports batch-level characterization and variability-aware quality prediction, improving logistics and operating-window selection. For process development, surrogate models and multi-objective optimization emerge as effective tools to navigate yield–cost–energy–sustainability trade-offs and to speed scale-up decisions under sparse data. At operation, digital twins and adaptive control, including reinforcement learning, strengthen robustness to disturbances and performance drift. Commercially, natural language processing (NLP) and network analytics enable quantitative market intelligence by mining patents, literature, consumer discourse, and regulatory texts to map trends, competitors, "white spaces", and adoption barriers. Across applications, the review identifies data governance, transferability, interpretability, and rigorous validation as the main deployment bottlenecks, and outlines a roadmap toward deployable AI-assisted business strategies in circular bioeconomy markets.

Keywords: agri-food waste valorisation; artificial intelligence (AI); predictive analytics; digital twins; techno-economic analysis (TEA); uncertainty quantification

1. Introduction

Agri-food waste and by-products refer to leftovers from food production, processing, and consumption that are discarded, even though they may still have nutritional value or potential for product development. This includes vegetables and fruit with dimensions or shapes rejected by the market, fruit peels, stems, and certain food scraps. The valorisation of these streams is increasingly framed within circular-economy and Sustainable Development Goals (SDGs)-oriented approaches, spanning the recovery of functional compounds and their re-use in foods, packaging, cosmetics, and other value chains [1,2]. Cultural attitudes towards food are very important; in many societies, there is a stigma attached to "scraps" or "leftovers", which can make it harder for consumers to accept products made from food waste. However, younger generations, especially those interested in sustainability, may be more open to trying new, unconventional foods, potentially leading to a shift in acceptance over time. Consumers generally care greatly about the safety and quality of the food they eat. When it comes to food made from agricultural by-products, the biggest hurdle is often overcoming doubts about safety and quality. Evidence from a recent scoping review on upcycled foods indicates that acceptance is strongly influenced by product-related cues and trust signals, including the presence of logos, labels, and certifications, alongside factors such as food-technology neophobia and environmental awareness [3]. Clear labelling and certification, together with effective communication demonstrating that products derived from food waste are properly processed and meet food safety standards, could therefore help increase acceptance. Transparency about how the product is made (for example, sustainable processing methods) can also help build trust, and recent work discussing commercialization of upcycled foods highlights that verified supply chains and unified certification/labelling frameworks are key enablers for scaling and credibility [4]. Many consumers are also looking for ways to reduce their carbon footprint, and products made from agri-food waste can be marketed as more sustainable options because they contribute to reducing food waste, which is a major environmental issue. Successful marketing campaigns that educate consumers about the benefits of using agri-food waste could play a significant role in increasing acceptance, including narratives about how waste is repurposed into valuable products, the environmental impact of reducing food waste, and how these products can match conventional alternatives in quality and safety [3,4].

The preliminary activities before developing any entrepreneurial business plan include assessing feedstock availability, with annual or seasonal volumes, as well as their general characteristics. It is essential to identify the type of waste and by-product, their composition, and in particular the water content, which strongly affects storage. Water content controls microbial growth, enzymatic activity, and chemical degradation; more broadly, food spoilage and safety risks are driven by interacting microbial, enzymatic, and chemical mechanisms that are highly sensitive to storage conditions [5]. High moisture accelerates spoilage, fermentation, and loss of functional compounds, potentially increasing safety risks and shortening shelf life. In stored commodities, moisture is also a critical co-factor (with temperature and humidity) influencing fungal growth and mycotoxin-related hazards, reinforcing the need for moisture-aware handling and stabilisation strategies [6]. Appropriate drying is therefore mandatory, avoiding harsh conditions that may induce structural collapse, oxidation, or loss of volatile compounds. Before any physical treatment, chemical composition and target compounds must be quantified. This is fundamental to determine the percentage of the most valuable compounds, including both primary and secondary metabolites, and to define feasible recovery routes in a circular-valorisation framework [1]. Lab-scale research can provide the data needed to design a reasonable potential exploitation of agri-food waste and by-products. The selected technologies for extraction, downstream processing, and purification must be scaled up at pilot scale to confirm yields and calculate energy consumption. In the case of a positive outcome, process engineers can design a semi-industrial plant for preliminary production. Finally, emerging technology families (e.g., advanced materials and nano-enabled solutions) are increasingly discussed as cross-cutting enablers for circular food systems, including preservation, waste valorisation and resource recovery, while also raising governance and safety considerations [7].

2. Top-Down and Bottom-Up Strategies

Top-down strategies for the valorisation of agri-food wastes and by-products are primarily driven by government policies, financial incentives, and market demand. These factors create a supportive framework for large-scale implementation of waste reduction and valorisation efforts. Such initiatives focus on regulation, incentives, and infrastructure development to drive the transition towards a circular economy [8]. This strategy is also guided by market analysis (market size, growth rates, and benchmarking against competing products). Currently, demand for vegetal proteins is increasing steadily, as is demand for soluble fibres such as beta-glucans and arabinoxylans. Similar trends are observed for bioactive compounds such as polyphenols, essential oils, and pigments.

Top-down strategies include regulatory instruments (e.g., separate collection mandates, landfill diversion targets, extended producer responsibility, and safety standards), financial mechanisms (subsidies, tax incentives, green public procurement), and infrastructure investments that reduce transaction costs across the supply chain. In AI-enabled business planning, these elements can be operationalized via policy and regulatory intelligence (NLP-based monitoring), scenario forecasting, and constraint-aware optimization that incorporates compliance and incentive structures.

These strategic layers define the boundary conditions for AI-assisted decision support: policy instruments shape objective functions and constraints (e.g., diversion targets, carbon pricing, compliance), whereas bottom-up operational heterogeneity determines the required feature set and robustness (seasonality, supplier effects, and quality uncertainty).

Bottom-up strategies for agri-food waste management are driven by producers (industries, farmers, local communities) and supply-chain actors [9]. These approaches focus on practical, localised, and context-specific solutions, often leveraging short logistics and decentralised pre-processing (e.g., stabilisation, drying, ensiling, or fermentation) to manage seasonal throughput and quality variability. They are typically supported by local partnerships and contractual specifications on minimum volumes and quality thresholds. In this setting, AI is particularly relevant for rapid intake characterization, supplier/batch risk scoring, and data-driven blending and scheduling decisions under heterogeneous feedstock availability. For example, there is large availability of specific by-products such as grape pomace and seeds, and orange, tomato, or potato peels.

3. Learning from Successes and Failures

Several examples of scale-up and commercialisation failures in agri-food waste and by-product valorisation reveal recurring technical and economic bottlenecks. Failures have occurred when the adopted technology, logistics costs, quality variability, and thin margins were underestimated [10]. Pipeline Foods, which focused on grain aggregation and traceability in the organic supply chain, illustrates how scale and working capital requirements can overwhelm a model even when demand signals are present. The seasonality of several matrices and competing uses reduces reliable throughput and product consistency, while feedstock risk due to heterogeneity and potential contamination (pesticides, mycotoxins, etc.) further complicates the process.

Dewatering, stabilisation, drying, and odour control are often significant cost drivers, especially for wet, microbially labile streams. The cost of drying water-rich plant matrices can be particularly high. This is the case with okara, a waste product from soy processing which, although rich in protein, soluble fibre, and mineral salts, is a gel containing over 80% water, making its recovery prohibitively expensive unless stabilisation and valorisation routes are carefully selected. In contrast, grape pomace can be transformed into valuable resources by extracting bioactive compounds (polyphenols, antioxidants) for functional foods, nutraceuticals, colourants (enocyanins), cosmetics, and animal feed, while also producing biofuels (ethanol), enzymes, and organic acids via microbial fermentation, thus promoting a circular economy and reducing waste. Noteworthy is the recovery of oil and proteins from grape seeds.

Scaling up from laboratory or pilot trials to industrial production is dominated by coupled technical and financial risks, where small deviations in yield, uptime, and utility demand can overturn the business case. A recurrent cost driver is energy intensity, especially for water-rich matrices requiring dewatering, stabilisation, or drying; in these cases, the cost of evaporation and heat integration may exceed the value captured if product selection and logistics are not optimized. Beyond utilities, commissioning and ramp-up frequently involve longer-than-expected learning curves: equipment tuning, control-loop stabilisation, cleaning cycles, and operator training can reduce early-stage capacity utilization and delay revenues while fixed costs remain high. Performance drift during scale-up can further reduce yields due to mass/heat-transfer limitations, mixing non-idealities, fouling, solvent recovery constraints, or variability in feedstock composition, leading to batch-to-batch inconsistency and higher downstream purification loads. Maintenance intensity and unplanned downtime increase unit cost through lower effective operating hours and higher labour and spare-part requirements.

Commercial viability also depends on bankable long-term agreements and clear regulatory pathways (food/feed/fertiliser/cosmetic claims), which require traceability, specifications, and quality assurance plans aligned with the intended market. Accordingly, cost accounting should be expressed in decision-relevant terms (most commonly cost per kg of ingredient delivered at specification, including utilities, yield losses, purification, waste handling, and logistics) since this metric directly sets the feasible selling price and margin.

Artificial intelligence can reduce scale-up risk by enabling uncertainty-aware modelling of yields and utility consumption through surrogate models and multi-fidelity strategies that combine data from different scales. In parallel, digital twins support ramp-up by continuously reconciling model predictions with plant data and allowing early detection of performance drift. Predictive maintenance mitigates operational risk by anticipating equipment failures and reducing unplanned downtime. Finally, coupling process uncertainty with scenario-based techno-economic analysis (Monte Carlo simulation and sensitivity assessment) helps identify the main drivers of €/kg production cost and prioritize targeted data acquisition and mitigation actions before committing to full-scale CapEx.

4. Best Available Technologies

Extraction and purification routes should be selected and justified based on the target product portfolio, feedstock properties, intended market (food/feed/cosmetics/materials), and process maturity (TRL). In practice, solvent choice, energy demand, safety constraints, and downstream separations often dominate unit cost and determine scalability. Recent circular-bioeconomy roadmaps emphasize process intensification, greener processing, and integrated, modular biorefinery schemes that can tolerate heterogeneous agri-food residues while maintaining product consistency [11,12].

4.1. Process Intensification

Ultrasound-assisted extraction (UAE) can reduce extraction time and solvent use by enhancing mass transfer, but industrial viability depends on robust continuous or semi-continuous operation and control under variable slurries. Cavitation-based systems (including hydrodynamic cavitation and rotor–stator devices) are attractive for scale-up due to continuous-flow compatibility and high throughput, though erosion, residence-time control, and variable rheology must be managed. Microwave-assisted extraction (MAE) offers rapid heating and accelerated kinetics, but scale-up requires designs that avoid non-uniform treatment. Pressurized liquid extraction (PLE) and subcritical water extraction (SWE) can provide high yields in short times and reduce organic solvents; however, lower selectivity may generate broad phytocomplexes or partial hydrolysis, which can be beneficial or detrimental depending on the target. Supercritical CO_2 (SC-CO_2) remains a key option for high-quality, low-residue fractions (notably lipids and aroma-related compounds), but higher CapEx and operational complexity typically confine it to premium products [13].

4.2. Downstream Processing

Downstream operations frequently determine cost per kg of ingredient at specification; therefore, extraction should be designed together with concentration and purification. Membrane separations (MF/UF/NF/DF) enable scalable fractionation and concentration in aqueous systems, often reducing thermal load compared with evaporation, but fouling and cleaning protocols are central design constraints. For higher-value fractions, adsorption resins or chromatographic polishing may be used to improve purity and standardization, albeit with potentially significant cost contributions. Precipitation/crystallization routes remain industrially established for proteins and some polysaccharides but require careful integration with solvent recovery and impurity control.

4.3. Bioconversion and Hybrid Routes

Biological conversion and hybrid schemes (extraction coupled with enzymatic upgrading or fermentation) are increasingly used to stabilize wet streams and expand product portfolios, particularly in “zero-waste” valorisation concepts [11]. Enzyme-assisted extraction (EAE) can enhance release under mild conditions, while fermentation can upgrade carbohydrate-rich residues into organic acids, bioalcohols, enzymes, and microbial biomass; both routes require attention to feedstock variability, hygienic control, and downstream design.

4.4. Materials Valorisation

For high-volume lignocellulosic residues where variability limits premium ingredient markets, biocomposites provide a robust outlet. Performance engineering through preprocessing (drying, milling, particle-size control) and fiber–matrix adhesion strategies can improve reproducibility and durability under variable feedstocks [14].

In an AI-focused perspective, these technologies define alternative valorisation routes whose suitability depends on feedstock attributes (e.g., moisture, composition, and variability) and target-market specifications. AI-enabled decision support is therefore most relevant at the screening stage, where predictive models fed by rapid sensing and historical performance data can rank feasible routes, flag out-of-distribution batches, and guide pilot-test prioritization. In addition, surrogate-based multi-objective optimization can support early trade-off analysis (yield/purity versus energy/solvent use and cost), improving route selection before detailed scale-up and investment assessment.

5. Product Classes from Agri-Food By-Products and Value-Driven Applications

Agri-food by-products can be transformed into marketable products through valorisation pathways that target either high-volume ingredients (typically primary metabolites and structural fractions) or high-value specialty ingredients (often secondary metabolites and enriched phytocomplexes). Across these product classes, economic viability is governed by a small set of recurring determinants: (1) feedstock variability (seasonality, composition, moisture, contamination risk); (2) process selectivity and stability (yield versus degradation/denaturation, reproducibility, and downstream separation burden); (3) specification compliance for the intended market (food/feed/cosmetic/material claims); and (4) the resulting €/kg-at-specification cost, which ultimately determines feasible pricing and margins.

Within an AI-assisted business-planning perspective, these product classes are best treated as decision options: AI-enabled sensing and predictive models support batch-level classification and quality estimation; surrogate modelling and optimization support route selection and operating-window design; and NLP-based market intelligence can monitor evolving claims, competitors, and regulatory constraints to guide positioning and partnership strategy. The following sections summarize the main product families, their applications, and the key decision trade-offs relevant to AI-enabled opportunity identification.

5.1. Primary Metabolites

Primary metabolites underpin scalable valorisation because they are often recoverable at meaningful volumes from widely available side-streams. Their market value depends not only on yield, but on functional performance (e.g., solubility, emulsification, viscosity) and on the ability to maintain batch-to-batch consistency under heterogeneous feedstock supply.

5.1.1. Proteins and Peptides

Proteins and peptides are in high demand globally and can be recovered from broken legume residues, oilseed meals, cereal by-products, and selected animal by-products (e.g., proteins from bones and tendons). Applications include food ingredients, human and animal nutrition, sports nutrition, and biodegradable materials. Their value is enhanced by techno-functional properties (solubility, foaming, emulsification, gelling) and bioactivity, but profitability is often set by the trade-off between extraction yield and loss of functionality induced by harsh conditions and extensive purification.

Protein recovery from deoiled seeds is a growing industrial route, commonly based on alkaline solubilisation followed by isoelectric precipitation (e.g., solubilisation at pH 9–11 and precipitation near pH 3.0–4.5), including intensified variants such as ultrasound-assisted alkaline extraction prior to precipitation [15]. While established, this approach may cause partial denaturation and lysine loss. An alternative is subcritical water extraction (SWE), where temperatures around 130–150 °C enable protein solubilisation without added chemicals; however, partial hydrolysis and reduced selectivity can affect functional properties, yielding broader phytocomplex fractions [16]. Aqueous enzymatic extraction promotes cell wall degradation and enhances protein release under milder conditions, improving functionality but often at higher cost and longer processing times. Efficient downstream processing by membrane fractionation (ultra- and diafiltration) can significantly increase purity, enabling use in food formulation, feed, and biomaterials.

AI can support rapid prediction of protein content and functionality from spectroscopy/imaging proxies, optimize extraction conditions (pH, temperature, time, solvent/enzymes) via surrogate models, and enable batch-to-batch QA through classification and anomaly detection.

5.1.2. Carbohydrates, Dietary Fibres, and Oligosaccharides

Dietary fibres and oligosaccharides derived from cereal brans, fruit residues, and vegetable wastes are important ingredients for low-glycaemic products and as prebiotics. Applications include gut-health ingredients, fat replacers, and texture modifiers. Their market value is supported by strong nutritional positioning, but technical value is highly dependent on molecular-weight distribution and process history, which shape rheology, water-holding capacity, and fermentability. Pectins and soluble fibres (e.g., beta-glucans and arabinoxylans) are particularly relevant for food structuring and formulation.

AI can learn structure–property relationships, predict rheological behaviour, and accelerate formulation and process screening under constraints (clean-label, allergen, cost), using optimization and active learning.

5.1.3. Lipids and Specialty Oils

Lipids and specialty oils are obtained from seeds, kernels, and processing residues. Main applications include food, nutraceuticals, cosmetics, and oleochemicals. When the unsaponifiable fraction is enriched in PUFA, phytosterols, or tocopherols, value is significantly increased. Across markets, oxidative stability and contaminant profiles strongly determine product acceptance and pricing.

AI can support impurity and stability prediction, accelerated shelf-life modelling, and market price forecasting to guide product positioning, quality strategy, and contract design.

5.2. Secondary Metabolites

Secondary metabolites generally deliver the highest value per kg, but they require more selective extraction, stability management, and stronger evidence for claims and safety. They are typically sourced from fruit peels, pomace, seeds, skins, leaves, and fermentation-derived streams [17].

Polyphenols comprise a large family including flavonoids (flavonols, flavones, catechins), phenolic acids, stilbenes, and lignans. Applications include nutraceuticals, functional foods, cosmetics, and active packaging, with value driven by health positioning, oxidative stability, and clean-label demand [18]. Natural pigments and colourants are also of strong industrial interest: carotenoids, anthocyanins, and chlorophylls extracted from peels, pomace, and leaves are used in food, cosmetics, and textiles as substitutes for synthetic dyes [19]. Aroma compounds and essential oils can be recovered by hydrodistillation of inflorescences, leaves, or fruit peels; flavour precursors can also be recovered from fermentation streams and peels, targeting food, beverages, and fragrances where low dosage and "natural" labelling command premium margins.

Beyond classic ingredient markets, several secondary-metabolite-rich fractions are commercialized as phytocomplexes, especially for cosmetic and pharmaceutical uses (anti-ageing, anti-inflammatory, antimicrobial formulations). Agronomic applications are also expanding, with biofertilisers, biostimulants, and biopesticides derived from extracts and hydrolysates that show functional activity and support sustainable agriculture [20].

Platform chemicals, bio-based solvents, and surfactants require higher specialization and open opportunities for green chemistry. A high-strategic example is 2-methyloxolane, a renewable solvent derived from cellulose (e.g., sugarcane bagasse), positioned as a safer alternative to petroleum solvents such as hexane, particularly for oil extraction [21,22].

AI-assisted spectroscopy can enable rapid quantification and detection of degradation/contamination; predictive models can optimize recovery while minimizing loss of activity; and NLP-based intelligence can track emerging claims, regulatory constraints, and competitive landscapes for these ingredient classes.

5.3. Most Valuable Products and Applications

Overall, the most valuable products recovered from agri-food by-products include both primary and secondary metabolites. The highest economic value is typically associated with bioactive compounds (polyphenols, flavonoids, carotenoids, tocopherols, phytosterols) used in food, nutraceutical, cosmetic, and pharmaceutical applications, where pricing is driven by claims, purity, and standardization. In contrast, production volumes are generally higher for dietary fibres (soluble/insoluble), pectins, beta-glucans, arabinoxylans, and oligosaccharides applied as functional ingredients and texture modifiers.

From a business-planning standpoint, product selection should be framed as a portfolio decision balancing: (i) premium markets with tighter specs and higher downstream cost; and (ii) bulk markets where throughput and logistics dominate. Fermentable substrates (sugars and polysaccharides) remain attractive for bioethanol, other bioalcohols, organic acids, and microbial biomass; mineral- and ash-rich fractions can be exploited for fertilisers, soil conditioners, and feed supplementation.

Finally, residual plant fibres from agri-food by-products are suitable sources for biocomposites and biopackaging due to abundance, renewability, and functional properties. Key components (cellulose, hemicellulose, lignin) provide mechanical reinforcement, barrier properties, and thermal stability. Plant fibres can act as fillers or reinforcements in PLA, PHA, starch-based, or protein-based matrices to improve stiffness and strength while reducing cost and carbon footprint. Surface modification and hybrid formulations are key strategies to overcome interfacial limitations and achieve industrial performance [14,23].

6. Artificial Intelligence in Agri-food Waste Valorisation: Advanced Methodologies and Implementation Strategies

The application of artificial intelligence to the valorisation of agri-food residues transcends conventional data analysis, offering instead a comprehensive framework that integrates predictive modelling, optimization algorithms, and decision support systems across the entire value chain. The inherent complexity of transforming heterogeneous biomass streams into consistent commercial products demands computational approaches capable of managing multidimensional uncertainty while extracting actionable insights from incomplete or noisy datasets. This section explores the technical architecture, algorithmic foundations, and practical implementation strategies that enable AI-driven transformation of agri-food waste management from an empirical craft into a data-informed industrial process. To provide an integrated overview of how artificial intelligence supports agri-food waste valorisation across multiple decision layers, Figure 1 summarizes the conceptual architecture adopted in this work. The framework highlights the interplay between data acquisition, predictive analytics, process optimization, digital twins, market intelligence, and techno-economic assessment, emphasizing how these components jointly enable uncertainty-aware and data-informed decision-making along the entire value chain.

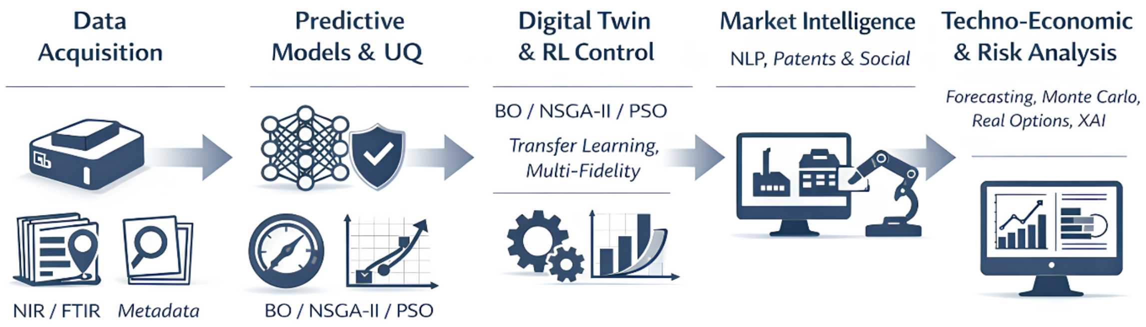

Figure 1. Conceptual architecture of an AI-driven framework for agri-food waste valorisation. The figure illustrates the integration of heterogeneous data acquisition (spectroscopic, visual, and contextual metadata) with predictive models incorporating uncertainty quantification (UQ), process optimization and scale-up strategies, digital twins with reinforcement learning-based control, market intelligence analytics, and techno-economic and risk assessment. Together, these components support data-informed decision-making across the entire valorisation value chain, from feedstock characterization to strategic and economic optimization.

6.1. Predictive Analytics for Feedstock Characterization and Quality Management

The central challenge in agri-food waste valorisation is the strong variability of incoming biomass, driven by differences in cultivation practices, harvest timing, storage, and prior processing. This heterogeneity introduces uncertainty that can propagate through downstream operations and compromise process stability and product consistency.

To illustrate the magnitude of feedstock heterogeneity at intake, Table 1 reports representative moisture contents (wet basis) for common agri-food residues/by-products. Moisture is a first-order driver of storability, microbial spoilage risk, transport economics, and the energy penalty associated with thermal stabilisation (e.g., drying or concentration).

For example, citrus residues and potato peels typically enter processing with very high water content, whereas dried pomace powders can be comparatively shelf-stable but still require moisture control to avoid caking and quality drift. The values reported for okara, grape pomace, potato peels, orange pomace, and carrot pomace are taken from the corresponding sources and compiled in Table 1 [24–28]. This table is included to quantify a first-order driver of variability (moisture) that directly impacts logistics, stabilisation energy, and operability, thereby motivating AI-enabled rapid sensing and predictive analytics at intake.

Table 1. Reported moisture content of selected agri-food residues/by-products (wet basis).

Residue/By-Product	Moisture Content (% w.b.)	Design Note (Why It Matters)	Reference
Okara (fresh soy pulp)	76–80	Very high water activity → rapid spoilage; typically requires immediate stabilisation (drying, fermentation, or cold chain).	[28]
Grape pomace (fresh; Benitaka cultivar)	75.7	High moisture → fast microbial growth and mass/heat-transfer limits; drying or ensiling often needed prior to extraction/storage.	[25]
Potato peels (raw)	83.3–85.1	Extremely wet matrix → high specific energy for evaporation; affects logistics and reactor residence times.	[27]
Orange pomace (fresh)	≈91.2	Very high initial moisture → drying is energy-dominant step; motivates multi-stage or low-temperature drying and valorisation close to source.	[24]
Carrot pomace powder (dried)	6.28–7.12	Low moisture → storage-stable ingredient; monitoring still needed to prevent caking and quality drift.	[26]

From an AI deployment perspective, the spread in moisture values implies that "one-size-fits-all" operating windows are rarely robust: identical equipment settings can lead to different effective solids loading, rheology, and heat/mass-transfer behaviour across batches [24,27]. Practically, this motivates (1) rapid at-line/inline sensing (e.g., NIR/FTIR or hyperspectral proxies) to estimate key quality attributes in near real time; and (2) uncertainty-aware models that flag out-of-distribution batches for additional testing or conservative operating policies. Because full laboratory characterization of every batch is often too slow and expensive at industrial scale, machine learning enables an alternative workflow: fast, non-destructive measurements are combined with historical datasets to deliver near–real-time estimates of composition and quality [29], ideally accompanied by confidence information.

Building reliable predictive models starts with broad, multi-source data acquisition. Spectroscopic signals such as near-infrared (NIR) and Fourier-transform infrared (FTIR) provide rapid proxies for major constituents and molecular features, while visible spectroscopy contributes information linked to pigments and related quality markers. When these measurements are augmented with contextual metadata (e.g., geographic origin, harvest date, storage duration, and supplier identity) the resulting feature space becomes high-dimensional, making feature selection and dimensionality reduction important to improve robustness and generalization [30].

Several modelling families are commonly adopted. Random Forests are frequently effective because they handle nonlinear relationships, reduce overfitting through ensembling, and provide interpretable indicators of which variables or spectral regions drive predictions. Gradient-boosting approaches (including XGBoost) often achieve high predictive accuracy by iteratively correcting residual errors, but they typically require careful hyperparameter tuning to balance performance and generalization. Neural networks offer additional flexibility for capturing complex mappings, especially when adequate training data are available. In spectroscopic contexts, one-dimensional convolutional networks are particularly relevant because they exploit local correlations along the wavelength axis and can learn informative spectral patterns without relying exclusively on manual feature engineering [31].

Model assessment must be designed to reflect real deployment conditions and to avoid spurious performance gains. Beyond standard cross-validation, validation schemes should account for supplier- or season-specific structure and temporal effects, and the strongest evidence of robustness comes from external testing on independent regions, years, or production campaigns. Practical deployment also raises the issue of instrument and condition variability: calibration transfer techniques allow models trained on one spectrometer or measurement setup to remain accurate when applied across other devices or sites, reducing the need for repeated, costly recalibration.

Extending predictive capabilities beyond chemistry, computer vision can capture morphological and visual quality attributes that affect processing efficiency. Convolutional models can support tasks such as defect grading, detection of foreign materials, ripeness estimation, and identification of disease symptoms, often leveraging transfer learning from pre-trained architectures. Hyperspectral imaging further combines spatial and spectral information into data cubes, enabling detection of localised contamination, inhomogeneity, or degradation that may be missed by bulk measurements; specialized deep learning approaches can integrate both spatial and spectral dependencies [32].

Finally, uncertainty quantification is essential for industrial decision-making, where incorrect predictions can have significant economic consequences. Probabilistic modelling, ensemble strategies, and distribution-free methods such as conformal prediction can provide prediction intervals or confidence measures, helping operators distinguish reliable estimates from cases where the model is likely extrapolating beyond its training domain.

6.2. Process Optimization and Intelligent Scale-Up Strategies

Scaling laboratory extraction methods into economically viable industrial operations poses a complex optimization problem involving many interacting process variables, hard physical constraints, and objectives that often conflict (e.g., maximizing yield while reducing energy use, processing time, and quality losses). Classical design-of-experiments remains valuable, but the number of required trials grows rapidly as the number of factors increases, making exhaustive exploration impractical for real, high-dimensional processes. AI-based optimization strategies address this limitation by searching large parameter spaces more efficiently and by making trade-offs between competing targets explicit [33].

A widely used approach for expensive pilot-scale experimentation is Bayesian optimization, which treats the process as a black-box function and builds a surrogate model to approximate the response surface from limited data. Gaussian process models are commonly adopted as surrogates because they provide both a mean prediction and an uncertainty estimate, which is critical when deciding where to sample next [34,35]. Acquisition rules then guide sequential experimentation by balancing exploitation of currently promising settings with exploration of regions where uncertainty is high and better solutions may exist [36].

From an implementation standpoint, Bayesian optimization typically begins with an initial set of diverse experiments designed to cover the feasible domain. It can also be adapted to practical constraints by proposing multiple experiments in parallel while discouraging redundant evaluations, and by incorporating contextual inputs (such as feedstock batch descriptors) so the optimizer can learn how optimal operating conditions shift as raw material properties change.

Because industrial design rarely optimizes a single outcome, multi-objective methods are often required. In this setting, solutions are evaluated through Pareto optimality, producing a frontier of operating points that represent different compromises among objectives. Evolutionary algorithms such as NSGA-II are commonly used to approximate this frontier by combining selection, crossover, and mutation with non-dominated sorting to maintain a diverse set of trade-off solutions. Multi-objective Bayesian optimization extends the same logic to scenarios where experiments are costly, using surrogate models for each objective and selecting new trials based on criteria that improve the Pareto set while accounting for uncertainty.

Population-based metaheuristics provide additional tools when the response landscape is highly non-convex or contains many local optima. Particle swarm optimization, inspired by collective movement in nature, explores the search space through a group of candidate solutions that learn from both individual progress and the best solutions found by the swarm. By tuning how strongly particles follow their own experience versus the swarm's global knowledge, the method can balance broad exploration with focused refinement, and adaptive variants can adjust this behaviour as the search converges.

Surrogate modelling is not limited to Gaussian processes. Deep neural networks can serve as flexible approximators when process behaviour is complex, non-stationary, or difficult to capture with standard kernels. While neural surrogates do not naturally provide the same principled uncertainty estimates as Gaussian processes, uncertainty can be approximated through ensembles of independently trained networks or through stochastic inference techniques (e.g., using dropout during prediction) to obtain variability estimates that support risk-aware optimization.

Knowledge transfer across scales is another core need in scale-up. Transfer learning and domain adaptation allow models trained on abundant laboratory data to inform pilot or industrial predictions, while adjusting for systematic differences between scales (including heat and mass transfer effects that shift apparent kinetics). Multi-fidelity optimization formalizes this idea by combining low-cost, lower-fidelity information (lab trials or simplified models) with limited high-fidelity pilot data, allocating experimental effort where it yields the highest expected value.

Mechanistic understanding can further strengthen optimization by embedding physics and chemistry directly in the modelling loop. Differential-equation-based models capture conservation laws and known kinetics, while hybrid approaches couple mechanistic "cores" with machine learning components that account for unmodeled effects, disturbances, or uncertain parameters. Physics-informed neural networks follow a related principle by training models not only to fit data but also to respect governing equations, which can improve extrapolation in regimes where data are sparse.

Digital twins integrate these elements into an operational framework: virtual replicas of extraction and purification systems that continuously update using sensor data [37]. In practice, twins often combine mechanistic models for well-characterized unit operations with data-driven modules for complex or poorly understood phenomena (e.g., fouling, foaming, or performance drift). Real-time state estimation methods support fault detection and predictive maintenance, while dynamic optimization routines adjust setpoints as conditions change. Reinforcement learning can be trained within these simulated environments to learn control policies before deployment, reducing commissioning risk and helping stabilize performance under feedstock variability and equipment degradation [38].

6.3. Market Intelligence and Strategic Positioning through Advanced Analytics

Market intelligence is a decisive pillar for the commercial viability of agri-food waste valorisation, because success depends on correctly reading market opportunities, competitive dynamics, regulatory evolution, and consumer acceptance. Compared with conventional research (surveys, focus groups, analyst reports), AI-driven approaches (especially NLP and social/network analytics) enable a continuous, data-rich, and quantitative monitoring of trends by processing large-scale corpora such as scientific literature, patents, regulatory texts, news, and social media [39].

A first stream of analysis is scientific literature mining (e.g., PubMed, Web of Science, Scopus), used to detect emerging technologies and application areas before they fully reach the market. Automated pipelines can apply named entity recognition to extract entities such as compounds, species, and processing methods, and relation extraction to infer links between waste streams and potential uses. Topic modelling (from classical LDA to neural topic models) supports mapping the thematic structure of research communities and tracking how attention shifts over time across different valorisation pathways.

In parallel, patent analytics provides forward-looking signals of industrial activity and strategic positioning [39]. Machine learning models trained on patent text and metadata can classify technology domains, infer applicant strategies, and approximate the likelihood of commercialization. Citation network analysis helps identify foundational patents and innovation trajectories, while semantic similarity and clustering highlight crowded areas versus "white spaces" with lower competition [40]. Adding geographic and temporal patterns of filings reveals regional specialization and investment momentum, guiding partnership, licensing, and market-entry decisions.

Recent progress in transformer language models (BERT-family architectures and derivatives) strengthens these tasks by improving classification, entity recognition, semantic search, and question answering. For technical domains, performance typically benefits from domain adaptation (continued pretraining/fine-tuning on specialized corpora) to better capture terminology and writing conventions in scientific, patent, and regulatory documents.

On the demand side, sentiment analysis applied to social media, e-commerce reviews, and online forums quantifies public perception of waste-derived products, sustainability claims, and brands. More granular aspect-based sentiment analysis decomposes opinions into components (e.g., taste, safety, environmental impact, value proposition), revealing which attributes drive acceptance or resistance. Temporal sentiment tracking supports rapid detection of shifts following launches, controversies, or regulatory announcements, enabling timely corrective actions [41].

To complement sentiment, topic modelling of consumer discourse identifies recurring concerns and information gaps, supporting targeted communication strategies. Comparing discourse across demographics and geographies exposes cultural differences in sustainability priorities, perceived risks, and readiness to adopt novel ingredients.

A further layer is network analysis of industrial and innovation ecosystems. By mapping collaborations and relationships, analysts can identify clusters, supply-chain structures, and competitive groupings. Knowledge graphs linking companies, technologies, products, and applications enable structured queries for partner discovery. Network measures such as centrality highlight influential actors, while structural hole/bridge analysis points to opportunities to connect otherwise separated communities and gain strategic leverage.

These components can be integrated into competitive intelligence synthesis, where heterogeneous signals are combined into profiles of competing initiatives (technology choices, target markets, funding, partnerships, commercialization progress). Predictive models can then estimate variables such as startup survivability or time-to-market using features like team composition, patent assets, funding history, and network position, supporting differentiation strategies and anticipation of competitor moves [42].

Finally, AI supports regulatory intelligence by continuously monitoring proposals, guidance documents, consultations, and enforcement signals. Classification can organize developments by jurisdiction, product category, and expected impact, while predictive approaches can estimate enactment likelihood and implementation timelines to enable proactive compliance planning.

Preference elicitation and choice analysis provide a structured framework to model consumer adoption patterns explicitly. By integrating responses from surveys, transaction records, and controlled experiments, techniques such as discrete choice analysis quantify the marginal value consumers assign to specific product features (including sustainability credentials, third-party certifications, or unconventional ingredient sourcing) thereby guiding both price optimization and formulation decisions. Machine learning-driven recommendation engines, leveraging both collaborative filtering and content-based algorithms, enable fine-grained audience segmentation and pinpoint which consumer cohorts demonstrate the highest propensity toward particular product configurations, ultimately enhancing marketing precision and optimizing resource deployment.

6.4. Economic Modelling, Risk Assessment, and Investment Decision Support

Economic success in agri-food waste valorisation depends on reliably estimating CapEx, OpEx, revenues, and risk over multi-year horizons under substantial uncertainty in feedstock availability, process performance, market prices, and regulation. Traditional discounted cash flow analysis is often built on fixed point assumptions, which can mask the probabilistic nature of key drivers and their interdependencies. AI-oriented approaches reframe financial evaluation as a dynamic, probabilistic decision-support system that: forecasts key variables; propagates uncertainty through the business case; identifies dominant risk factors; and supports strategy selection under multiple scenarios [43,44].

At the macro-scale, economic and risk assessment for valorisation projects is increasingly anchored to global baseline indicators on food loss and waste (FLW), because these values contextualize market size, policy pressure, and climate-related externalities. Table 2 summarizes widely cited global FLW indicators used in techno-economic screening and risk narratives (e.g., demand justification, avoided-emissions claims, and sensitivity bounds for feedstock availability and diversion potential) [45–48]. These global baselines provide the quantitative context for scenario definition (policy pressure, externalities, and addressable volumes) and motivate AI-assisted forecasting and uncertainty-aware economic evaluation rather than static, point-assumption business cases.

Table 2 is used to anchor AI-assisted decision support in economically meaningful baselines. These indicators motivate scenario-based modelling where AI forecasts key variables (e.g., demand and price trajectories) and uncertainty is propagated through techno-economic analysis (e.g., Monte Carlo and sensitivity) to identify dominant risk drivers. This links macro-scale FLW context to investment-grade decisions on route selection, scale-up timing, and risk mitigation. The baselines matter operationally for two reasons. First, they bound the "addressable" volume potentially available for diversion into higher-value pathways, while highlighting that interventions span both pre-retail losses and post-retail waste streams. Second, the reported climate and economic burdens motivate the inclusion of externalities (or policy-driven price signals) in scenario design, e.g., carbon costs, landfill restrictions, separate collection mandates, or EPR-type instruments, so that cash-flow models and Monte Carlo analyses reflect plausible regulatory trajectories rather than static assumptions [46,47].

Table 2. Global-scale baseline indicators relevant to economic and risk assessment of food loss and waste.

Indicator	Estimate	Reference Year	Primary Source
Food lost in the supply chain (post-harvest to before retail)	13.3% of food produced	2023	[45]
Food wasted at retail + food service + households	1.05 billion tonnes; ≈19% of food available to consumers	2022	[46]
Food waste breakdown by sector	Households: 631 Mt (79 kg/cap); Food service: 290 Mt (36 kg/cap); Retail: 131 Mt (17 kg/cap)	2022	[46]
Climate impact of food loss and waste	8–10% of annual global GHG emissions	n/a (annual estimate)	[47]
Economic cost of food loss and waste	≈USD 1 trillion annually (combined toll)	n/a (annual estimate)	[47]

The foundation of economic modelling relies on temporal forecasting of market demand trajectories, pricing evolution, and sectoral expansion rates. Traditional approaches like ARIMA models effectively capture serial dependencies and recurring patterns yet frequently falter when confronted with structural breaks and non-stationary behaviour characteristic of nascent market segments. Exponential smoothing frameworks employing state-space representations deliver reliable decomposition of trend and seasonal components while automating model specification procedures. Prophet emerges as particularly valuable for industrial applications due to its capacity to accommodate overlapping seasonal cycles, calendar-specific events, and abrupt trajectory shifts, proving especially effective when historical datasets span multiple years and exhibit pronounced cyclical characteristics.

To capture longer-range dependencies and nonlinear temporal patterns, LSTM networks provide a deep-learning alternative. Their gating mechanisms retain relevant historical information while filtering noise. For multi-step forecasting, strategies include recursive prediction (feeding forecasts back as inputs) and direct prediction (training separate models per horizon). Attention mechanisms can add interpretability by highlighting which past periods most influence the current forecast.

Because economic variables are interlinked, multivariate time-series modelling is critical. Demand for valorised ingredients, for instance, may co-move with meat prices, income trends, or competing products. Vector autoregression (VAR) and Bayesian VAR frameworks model joint dynamics; tools such as Granger causality help identify lead–lag relationships, and impulse response analysis quantifies how shocks to one variable propagate through the system.

A complementary pillar involves Monte Carlo methodologies for channelling parametric uncertainty through financial projection frameworks. Variables including raw material procurement costs, extraction efficiencies, utility expenditures, market valuations, and capital investment components are characterized through probabilistic distributions derived from retrospective datasets, specialist judgment, or comparative industry metrics. Triangular distributions prove suitable when boundary values and modal estimates are available, whereas lognormal specifications accommodate inherently positive variables exhibiting asymmetric upward dispersion. Iterative stochastic sampling generates empirical frequency distributions for key performance metrics including net present value and internal rate of return. These probabilistic frameworks surpass deterministic point estimates by explicitly quantifying both downside risk and upside opportunity. Correctly handling dependencies among inputs is essential: assuming independence when variables co-vary can distort risk estimates. Copula methods allow the joint distribution to be modelled by combining marginal distributions with a flexible dependence structure, including nonlinear and tail dependencies. Sensitivity analysis (e.g., rank correlation between inputs and outputs) identifies the variables that most drive financial performance, guiding data collection priorities and targeted risk mitigation.

Deep learning can enhance scenario generation and simulation speed. Neural surrogate models can approximate computationally expensive simulations, enabling faster or real-time what-if analyses [49]. Generative adversarial networks (GANs) can create realistic multivariate scenarios consistent with historical patterns and dependencies, while variational autoencoders (VAEs) can compress complex uncertainty into lower-dimensional latent representations that are easier to sample efficiently.

For strategic decisions that unfold over time, reinforcement learning (RL) provides a framework for sequential optimization under uncertainty. By formulating choices as a Markov decision process, RL algorithms learn policies that maximize long-term reward. Q-learning estimates values for state–action pairs, and deep Q-networks (DQN) extend this to high-dimensional settings, supporting decisions such as timing of capacity expansion, feedstock procurement policies, or portfolio evolution.

At the supply-chain level, uncertainty-aware optimization often uses stochastic programming, separating "here-and-now" decisions from "recourse" actions that adapt once uncertainty resolves. Two-stage stochastic programs evaluate first-stage decisions by accounting for expected costs of optimal second-stage responses across many scenarios. Scenario sets can be built via sampling or moment-matching into discrete scenario trees, and large problems can be solved efficiently using decomposition methods such as progressive hedging.

To value managerial flexibility, real options analysis complements standard NPV by capturing the option to delay, expand, abandon, or switch technologies as information evolves. Binomial lattice approaches discretize uncertainty into decision trees, and risk-neutral valuation can price options without explicitly specifying risk preferences. This perspective often shows why staged scale-up or modular configurations can be strategically superior to large, irreversible investments even if they appear less cost-efficient on paper.

Bayesian network architectures enable causal reasoning and holistic risk evaluation by encoding interdependencies among technical parameters, market dynamics, and economic indicators within directed acyclic graph structures. These frameworks facilitate dual-mode probabilistic reasoning: retrospective analysis identifying probable root causes underlying adverse performance, and prospective inference projecting outcome distributions given observable system states. Structure identification algorithms, whether score-optimization or conditional-independence approaches, can extract network topology directly from empirical data, occasionally uncovering non-intuitive correlations with material implications for uncertainty quantification and mitigation strategy formulation. Because stakeholders need transparency, explainable AI (XAI) methods such as SHAP and LIME help interpret complex models by attributing predictions to input contributions. Counterfactual explanations add an action-oriented view by identifying minimal changes to inputs that would meaningfully improve predicted outcomes, pointing to practical levers for performance improvement.

Finally, these tools are most valuable when integrated into a unified decision-support platform that links technical and economic evidence. Dashboards can display forecasts, uncertainty distributions, scenario comparisons, and key drivers; alert systems can monitor leading indicators and trigger contingency plans; and continuous-learning loops can update models as operational data accumulates, improving accuracy and decision quality from planning through construction and long-term operation [50].

6.5. Potential Challenges for AI-Assisted Business Strategies

Despite its potential, deploying AI for agri-food waste valorisation faces recurring challenges that can limit generalisation and business impact. First, data scarcity and bias are common because datasets are fragmented across sites, seasons, suppliers, and product specifications; this can lead to models that perform well retrospectively but fail under new campaigns. Second, non-stationarity and distribution shift (seasonality, climate effects, changes in preprocessing and procurement) require continuous monitoring, recalibration, and out-of-distribution detection to maintain reliability. Third, measurement and label uncertainty (noisy assays, inconsistent sampling, delayed ground truth) can propagate into predictions; uncertainty quantification and deployment-grade validation are therefore essential to avoid misleading recommendations. Fourth, operational deployment introduces integration and lifecycle burdens (sensor reliability, data pipelines, cybersecurity, and model maintenance) so robust MLOps practices are needed to keep models accurate after go-live [51]. Finally, in compliance-driven markets, interpretability, traceability, and auditability are critical to justify AI-supported decisions affecting safety, procurement, and regulatory alignment [52].

7. Conclusions

Agri-food waste valorisation requires robust market and investment decisions under feedstock variability, process uncertainty, and evolving regulation. This review contributes an integrated AI-enabled framework that links feedstock intelligence, process design and operation, market analytics, and uncertainty-aware investment assessment into a single decision workflow for valorisation projects. Specifically, sensing plus machine learning enables rapid intake characterization and variability-aware quality prediction; surrogate modelling and multi-objective optimization accelerate process design while making yield–cost–energy trade-offs explicit; and digital twins support adaptive operation under changing conditions. Commercially, NLP and network analytics extract actionable intelligence from patents, scientific literature, regulatory texts, and consumer discourse to improve opportunity identification, competitive "white-space" mapping, and strategic positioning. Investment appraisal benefits from uncertainty-aware techno-economic and risk analysis that replaces static assumptions with probabilistic decision support and highlights dominant risk drivers. Key deployment bottlenecks remain data governance and access, transferability across regions and waste streams, validation in real operating conditions, and interpretability/auditability for regulated markets.

Progress toward deployable AI-assisted business strategies will require shift-aware models with routine monitoring and recalibration across seasons and suppliers, together with stronger transfer learning across residues and regions. Multi-site evidence building will benefit from standardized data/metadata and privacy-preserving collaboration (e.g., federated learning) to reduce fragmentation. Hybrid and constraint-aware approaches that couple mechanistic knowledge with learning are expected to improve extrapolation and prevent infeasible recommendations. Finally, tighter integration of AI outputs with LCA/TEA and decision dashboards will enable portfolio-level route selection and staged scale-up under quantified uncertainty, supporting scalable circular bioeconomy business models.

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Use of AI and AI-Assisted Technologies

During the preparation of this work, the authors used AI-assisted tools, including OpenAI ChatGPT, to support language polishing, improve text fluency, assist in bibliographic scoping, and aid the preparation of the conceptual figure. These tools were used only as support. All scientific interpretation, critical evaluation of the literature, manuscript revision, and final approval were carried out by the authors, who take full responsibility for the content of the article.

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