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EXTRUSION SCIENCE AND TECHNOLOGY – PROCESSING AND PRODUCTS

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Review Based Book Chapter

**DATA-DRIVEN OPTIMIZATION OF SUSTAINABLE FOOD
AND FEED EXTRUSION: VALORIZATION OF AGRO-
INDUSTRIAL BY-PRODUCTS AND MACHINE LEARNING
APPLICATIONS**

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REVIEW BASED BOOK CHAPTER**DATA-DRIVEN OPTIMIZATION OF SUSTAINABLE FOOD AND FEED
EXTRUSION: VALORIZATION OF AGRO-INDUSTRIAL BY-PRODUCTS AND
MACHINE LEARNING APPLICATIONS**

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Abstract

Extrusion is a versatile thermomechanical technology with considerable potential for transforming agro-industrial by-products into value-added food and feed products. However, the complex interactions among raw-material composition, moisture, temperature, screw speed, mechanical energy, and equipment configuration make extrusion inherently nonlinear and difficult to optimize using conventional trial-and-error approaches. This chapter examines sustainable food and feed extrusion from an integrated perspective, linking the valorization of cereal, fruit, legume, and oilseed-derived by-products with the physicochemical transformations and functional properties generated during processing. Particular attention is given to the effects of extrusion on starch, dietary fiber, proteins, and lipids, as well as on hydration, expansion, bulk density, hardness, and digestibility. Traditional optimization through response surface methodology is discussed alongside emerging data-driven approaches, including artificial neural networks, Random Forest, XGBoost, and Bayesian optimization. These methods offer increased flexibility for capturing nonlinear interactions and supporting multi-objective optimization involving product quality, nutritional integrity, by-product inclusion, and resource efficiency. A structured framework for data-driven extrusion is presented, encompassing comprehensive ingredient characterization, robust experimental design, data preprocessing, model validation, and multi-objective optimization. Finally, the integration of predictive models, inline sensing, and intelligent control systems is discussed as a pathway toward adaptive and more resource-efficient extrusion. Combining extrusion technology with machine learning and rigorous data science can accelerate the transition from empirical process development toward

predictive manufacturing while supporting waste valorization and the principles of a circular bioeconomy.

Keywords

Extrusion Processing, Agro-industrial By-products, Circular Bioeconomy, Machine Learning, Response Surface Methodology, Bayesian Optimization, Artificial Neural Networks, Multi-objective Optimization, Process Digitalization, Waste Valorization

INTRODUCTION

Food extrusion is an established HTST (high temperature, short time) process in which traditionally low moisture ingredients are mixed, homogenized and shaped into intermediate or finished products by forcing them into an exit die of a specific shape and size. These ingredients typically include high starch and protein to produce a variety of RTE (ready to eat) food items, like snacks, cereals, pasta and pet food [1]. This process normally involves applying intensive energy under pressure for a short time to form viscous dough; the working time is just a matter of seconds, which allows for maintaining the properties of ingredients and bioactive compounds, while having a high rate of inactivation of microorganisms and anti-nutritional factors [2].

Despite offering many advantages to production lines, extrusion technology is often referred to as a “black box” system where the operating conditions and response relationships are difficult to predict. Optimizing an extrusion process poses a significant challenge due to its highly interdependent physicochemical transformations; additionally, the final product's properties are sensitive to the numerous processing parameters, such as temperature, moisture, screw speed, and the formulation itself. Singh et al. [3] demonstrated that feed moisture content significantly influenced the textural properties and amino acid profile of sunflower-incorporated meat analogues. Similarly, Pavani et al. [4] highlighted that barrel temperature played a more substantial role than screw speed in determining the nutritional qualities of pea protein isolate extrudates. Examples like these only investigate individual effects on individual properties, thus, the process of extrusion as a whole remains largely not understood fully. Conventionally, the primary approach to optimization of extrusion parameters has been Response Surface Methodologies (RSM), and while it has proven effective in various applications beyond extrusion, such as extraction and microencapsulation, RSM

has limitations. RSM relies on polynomial models that may oversimplify the nonlinearity and dynamic nature of the studied process and requires extensive experimental trial. Moreover, in the food industry, when dealing with pilot-scale processes, experiments demand substantial amounts of raw material, labor and experiment time. These constraints lead to the necessity for further look into advanced and adaptable optimization approaches to effectively reduce the so-called “trial-and-error” phase of a process, while maintaining a robust optimization.

One such approach is Bayesian Optimization (BO), a Machine Learning technique that has emerged as a promising alternative to traditional optimization methods [5]. This technique utilizes probabilistic surrogate models (like a Gaussian Process) to navigate complex parameter spaces efficiently. It is continuously refined with each new added data point and uses an acquisition function to guide the next most informative experimental condition. By adaptively suggesting experimental trials while capturing non-linear dynamics, BO offers a powerful framework for addressing the challenges inherent in extrusion processes [6].

Despite success in fields like 3D printing, BO remains largely unexplored for food manufacturing processes, presenting a chance for innovation. A recent study published by Theng et al. [7], demonstrated the effectiveness of this method in high-moisture extrusion optimization. They successfully modeled the relationship between key extrusion parameters (moisture content, barrel temperature, and screw speed) and textural properties including hardness, chewiness, springiness, and cutting force.

1. SUSTAINABLE RAW MATERIAL SELECTION

The inclusion of agro-industrial by-products is dependent on proximal composition as much as the type of product of interest. The extrusion process allows for texturization of proteins to a point where plant-based proteins can be transformed into a fibrous texture similar to that of meat. This way, it is possible to obtain products with similar sensory profiles to animal products. Extrusion changes the morphology of the fiber and reduces its size. Fiber-rich ingredients usually come from either cereal bran like wheat, rice, corn or oats, or fruit pomaces like apple and pineapple or mango and citrus' peels. In the final product, the extrusion process increases dietary fiber, resistant starches and

essential amino acids, by increasing bioavailability. Fiber content tends to positively influence hydration properties like water absorption and solubility indices; however, high fiber content also increases viscosity and modifies flow, while reducing starch gelatinization and expansion, leading to increased hardness. Therefore, fiber-rich ingredients require special attention to carefully adjust extrusion conditions for their use.

Alongside carbohydrate rich ingredients, protein-rich ingredients such as oilseeds have also been studied. Oilseeds are a diverse group of plant seeds with a long history of contributing to global agriculture and the food industry. They are also recognized as an excellent source of protein and as sustainable ingredients for plant-based diets [8]. Oilseeds are typically processed through pressing and/or organic solvents to extract their oils; this also creates a cake which may be further processed into a meal. Recently, there has been an interest in their derivatives as there is an increased awareness of their nutritional and functional benefits; benefits that have developed these protein-rich components beyond just byproducts and into novel ingredients for food and feed, while attending to a demand for sustainable sources of protein. Additionally, oilseed proteins have been linked to health benefits [9]. This, along with considerations associated with the ethic and environmental aspects of traditional animal protein have caused the demand for these plant-based ingredients to rise significantly [10].

However, while very rich in nutrients, these co-products are often limited to use in animal feed, due to the content of antinutritional and even toxic factors present in cakes and meals, such as oxalates or tannins, or the presence of allergens, as is the case for soybean or peanut [8].

Table 1. Characteristics, processing methods and applications of oilseed cakes, meals and proteins

Feature	Oilseed cakes	Oilseed meals	Oilseed proteins
Oil content	Highest residual (5-10%)	Lower residual oil (<2%)	Negligible oil content (highly defatted)
Protein content	Moderate (25-40%)	High (40-50%)	Very high (up to 90%, depending on purity)
Texture	Coarse	Fine	Powdered

Processing method	Mechanical pressing only	Mechanical pressing + solvent extraction	Further processing, such as protein isolation or concentration
Main components	Oil, fiber, and proteins	Proteins, fiber, minimal oils	Majority proteins, minimal fiber and oils
Applications	Animal feed, further processing	Animal feed, aquaculture, and other industrial applications	Food grade products: protein powders, plant-based meat alternatives and functional ingredients
Use in human nutrition	Limited	Occasionally processed for human consumption	Extensively used in food products
Examples	Soybean cakes, sunflower cake	Soybean meal, sunflower meal	Soy protein isolate, hemp seed protein concentrate

Extrusion technology presents a promising avenue for the further processing of these coproducts as a means of valorization; it offers a versatile and efficient way to enhance the nutritional and techno-functional qualities of oilseed proteins, thus expanding their applicability in various foods and feed formulations.

One of the most important by-products used in extrusion are oilseeds, such as soybean, sunflower seed, rapeseed and peanuts, among others. As of 2022, approximately 630 million metric tons of oilseeds were produced globally, with an additional 20 million in the year 2023 [11, 12].

These oilseeds have a variety of uses beyond their oil production: such as animal product alternatives like tofu and milk in the case of soybean, confectionery and snack foods for peanuts and as part of multigrain breads and breakfast cereals like flaxseed and sunflower seed. While many of these oilseeds are recognized as having attractive properties for novel formulations [13 -16], and presenting health benefits [8, 17, 18], many of the post-processing cakes and meals see limited use as simply feed for poultry and livestock species [14, 19]. Moreover, crops like hemp see additional hurdles in the

form of compliance to THC limits set regulatory bodies such as the USDA, Health Canada and European Commission.

2. SPECIALIZED APPLICATIONS

2.1. Production of functional foods through extrusion technology

Extrusion is already a well-established technology for the production of ready-made food products with improved structural, functional, sensory and organoleptic properties via thermomechanical treatments. These products are gaining popularity in the food industry due to the different ingredients that can be used and innovative new applications for value-addition of products.

2.2. Meat Analogues

These are defined as food products which mimic the aesthetic, sensory and chemical properties of conventional meat products [20]. Some of the most accessible ingredients for this type of product include low-cost cereals, pulses and vegetables. High moisture extrusion is extensively used to emulate the characteristic fibrous texture of meat with plant-based proteins. Chiang et al. [21] studied the effect of moisture content on the extruded meat alternatives made from Maillard-reacted beef bone hydrolysate with plant protein. Their results highlighted the critical role of moisture content as a process parameter in the formation of the fibrous structure in extruded meat alternatives.

Maillard reaction plays a critical role in volatile flavor compounds and cooked food. This reaction occurs between amino groups and reducing sugars under specific conditions, leading to the formation of Maillard reaction products [22, 23].

2.3. Fortification

Value-added food products can be developed through the extrusion process by utilizing food by-products from food processing industries.

Cereal flours can be enriched with fruit and vegetable by-products that are high in fiber, vitamins, and minerals. These byproducts are used to develop novel and innovative food products with functional properties. Much research has been done to analyze the effect of raw materials composition and extrusion parameters on the

functional and sensorial attributes of extruded food products, as the extrusion process significantly alters the total fiber content, starch, and protein digestibility [24]. The starch structure can be modified through extrusion to enhance the physicochemical and structural properties of snacks. Texturized rice can be produced using bran and broken rice through an extrusion process. The final product contains notable amounts of dietary fiber, protein, fat, thiamin, and riboflavin, making it nutritionally distinct from polished rice due to differences in physicochemical properties [25].

Mitrus et al. [26] studied the impact of extrusion-cooking conditions on the pasting characteristics of extruded white and red bean seed flour. Results indicated that gel formation ability in extrudates was decreased upon incorporation of white and red bean seed flour, attributing it to the high protein and fiber content of bean seeds. The pasting characteristics of their control sample (non-extruded beans) indicated that viscosity increased with increasing temperatures of 30-90°C but remained constant during the cooling stage. Similarly, increasing water inclusion had a positive impact on peak viscosity. Extruder screw speed also increased peak viscosity in the white bean. However, the red bean has a non-significant effect of screw speed on peak viscosity. Their results indicated that the retrogradation tendency of bean paste was reduced due to the degradation of starch materials during extrusion cooking.

García-Segovia et al. [27] studied the incorporation of insect and pea powders as alternative sources of protein and minerals in extruded snacks. Their results revealed that adding pea protein extrudate, *Alphitobius diaperinus* extrudate, and *Tenebrio molitor* extrudate increased protein content by 48.07%, 33.57%, and 25.73%, respectively. Ash content was also increased. Among the formulations, *Tenebrio molitor* powder-enriched extrudates had the highest selenium content, an essential trace element vital for human health. The study further found that the inclusion of insect and pea powders did not significantly alter the physicochemical and mineral properties of the snacks. Gumul et al. [28] studied the incorporation of various concentrations of apple pomace as health-promoting compounds in the production of corn snacks. Results indicated that apple pomace supplementation significantly increased the total polyphenol content by 79.0%. Similarly, the dietary fiber of gluten-free snacks increased

significantly with 20% apple pomace incorporation. Results revealed that phenolic acid increased significantly with apple pomace addition, such as cryptochlorogenic and chlorogenic acids. They concluded the best addition level was 20% due to its health-promoting characteristics observed in corn-apple snacks. Thus, the development of such snacks could be suggested on an industrial scale due to their best sensorial attributes.

Asif et al. [29] investigated the effect of including citrus pomace into corn grits to develop fiber-enriched extruded snacks. The inclusion of citrus pomace significantly increased total and dietary fiber, calcium content, and antioxidant activity, whereas it decreased expansion ratio, porosity, and oil absorption. Sensory evaluation showed that products containing up to 5% citrus pomace were well accepted. Similarly, Asif et al. [30] developed protein-enriched corn extrudates by incorporating chickpea flour at varying concentrations. Chickpea addition notably improved protein, dietary fiber, mineral content, and antioxidant capacity, along with enhanced bulk density and porosity. Sensory assessment revealed high acceptability at 60 g/kg inclusion. Overall, the incorporation of fruit by-products and legume flour into cereal-based extrudates effectively enhanced their nutritional, functional, and sensory properties, establishing their potential for developing sustainable and health-promoting snacks.

Valorization of agro-industrial byproducts such as fruit pomace, cereal bran and oilseed cake and meals promotes a circular economy [31]. However, sustainability in extrusion extends beyond product innovation to encompass energy efficiency, raw material utilization, and environmental impact. Optimizing screw design, barrel heating, and moisture control can reduce specific mechanical energy by 20–30% [32]. Novel techniques such as gas-assisted extrusion, including supercritical CO₂ and nitrogen-assisted systems, enables processing at lower temperatures, thereby preserving heat-sensitive nutrients and reducing energy demand [33]. Sustainable extrusion also includes water reuse, solvent-free formulations, and the development of biodegradable packaging materials [34]. Life-cycle assessments reveal trade-offs between reduced processing time and higher capital investment, highlighting the need

to integrate environmental, safety, and techno-economic assessments for large-scale adoption.

3. PHYSICOCHEMICAL TRANSFORMATIONS

3.1. Effects of extrusion processing parameters on nutritional values of extrudates

3.1.1. Starches

The extrusion process' high temperature and pressure cause changes in the starch structure, such as the loss of crystallinity and destruction of starch granules. The process can affect the pace and degree of starch digestion from a nutritional standpoint. This is because the structure of the starch molecules can be modified during extrusion, which can affect how easily they are broken down by enzymes in the digestive system. For example, extruded foods may have a higher degree of starch gelatinization, which can lead to more rapid starch digestion and absorption in the small intestine [35]. However, extrusion can also promote the formation of resistant starch, which is not digestible in the small intestine and functions more like dietary fiber. The balance between increased digestibility and resistant starch formation depends on the specific extrusion conditions used [36]. The features of starch digestion may be impacted by starch fragmentation during extrusion, particularly waxy starches. Dextrinized starch has a higher propensity for retrogradation because of its increased molecular mobility [37]. Wang et al. [38] reported that retrogradation during extrusion cooking can result in the formation of enzyme-resistant starch (RS) in cereals or cereal starches.

3.1.2. Dietary fiber

Dietary fiber is defined as edible carbohydrate polymers of ten or more monomer units that are not hydrolyzed by endogenous enzymes in the small intestine. Extrusion increases the solubility and availability of dietary fiber by breaking down the cell walls and other structural components of the material. Extrusion has been shown to increase the amount of soluble dietary fiber, which contributes to an overall increase in the total dietary fiber content. Research conducted by Sobota et al. [39] indicated that extrusion process tends to enhance the soluble fraction of dietary fiber content. Soluble

fiber is associated with cholesterol reduction, blood sugar regulation, and improved gut health, while insoluble fiber primarily aids in bowel regularity. In a different study, soluble dietary fiber (SDF) was improved from oat bran by using extrusion. In some cases, such as with barley flour, extrusion increased total dietary fiber content, with the increase attributed partly to a shift from insoluble to soluble forms, and partly to the formation of resistant starch and enzyme-resistant indigestible glucans through a process called transglycosidation [36].

3.1.3. Protein quality and solubility

Protein molecular structure is highly influenced by the different steps of extrusion (i.e., heating, mixing, and shearing). Throughout the process, proteins unfold, realign, hydrolyze, and denature [40]. As temperature increases during heating, hydrogen bonds break down, allowing protein chains to gradually unfold; at sufficiently high temperatures, intramolecular disulphide bonds are disrupted, as intermolecular disulphide bonds are formed. Shear forces caused by high screw speeds significantly affect protein interactions. They can act on the reduction of protein molecular weight and exposure of thiol groups of certain amino acids. However, screw speed also significantly affects residence time, making it difficult to isolate the individual contribution of shear alone.

A recent study showed that the extrusion process has improved the digestibility and availability of critical amino acids in food products. Extrusion may be an effective way to improve the nutritional quality of lentils and other legumes by increasing the availability and digestibility of essential amino acids [41]. In addition, extruded maize flour and soy protein concentrates significantly increased the biological value of proteins while maintaining the same levels of important amino acids, including accessible lysine [42]. Inactivation of anti-nutritional chemicals and the thermal denaturation of proteins have been identified as the main causes of improvement in digestibility after extrusion.

Protease inhibitors, which attach to enzymes such as trypsin and prevent them from digesting proteins, can also be found in legumes and cereals. It is possible to mitigate

the action of these interfering chemicals to improve protein digestibility, extrusion temperature combined with shear, often reach the denaturation conditions of these enzymes [43]. Because proteins make dough more viscous and inhibit flow in the extruder barrel, high-protein materials expand less during extrusion and produce less expanded products with increased hardness, which may negatively impact sensory acceptance [27, 44].

3.1.4. Lipids

During the extrusion process, proteins and starch can form complexes with lipids as a consequence of them forming an amorphous matrix, creating a variety of structures that can affect the nutritional and functional properties of the final product. The conformation of amylose changes to a monohelical structure, where the outside of the helix is hydrophilic and the inside hydrophobic. This allows free fatty acids, monoglycerides, and even aroma compounds to enter into this amylose helix. The formation of these complexes can have both positive and negative effects on the nutritional and functional properties of the final product. For example, unsaturated fats are more prone to oxidation, which leads to the formation of compounds perceived as rancidity in extrudates. The oxidative stability of the lipids is enhanced by their binding to starch. As a result, compared with lipids that are not bonded, a significant fraction of critical fatty acids will be maintained during extrudate storage. Lipids also generally act as lubricants during the extrusion process, lowering residence time and thus, the shear and temperature effects on the extrudate [45].

4. FUNCTIONAL PROPERTY EVALUATION

4.1. Effects of extrusion processing parameters on functional properties of the extrudates

4.1.1. Hydration properties

The hydration properties of extrudes can be measured from the water absorption and solubility indices (WAI and WSI, respectively). WAI measures the degree to which starch is gelatinized, affecting the sense of satiety extrudes give, while WSI measures the degree to which starch is degraded, affecting how digestible extrudates are [46]. This is

in part contributed to by the mechanical shear of the extrusion process, it works by disrupting the structure of starch granules and rupture of cell walls, exposing the hydrophilic groups of starch chains, as well as proteins, thereby improving water absorption and hydration capacities [47]. Water content is also a contributor, by affecting the swelling capabilities of starch granules to the point of breakage; this increases viscosity, which causes starch to behave as a thickening agent, limiting mechanical disruption [48, 49].

4.1.2. Expansion ratio and Bulk density

Bulk density is interdependent with the expansion index, the increased in bulk density will correspond to a decrease of expansion index and vice versa. In extruded materials, the expansion ratio is an important characteristic linked to the interaction between starch and proteins, and is an important sensory property, as it is the main factor influencing crispiness and mouthfeel. The expansion of the extruded products is influenced by various factors, including barrel temperature and especially feed's moisture content. When the barrel temperature increases, the water inside the feed material enters a superheated state, causing a violent burst of steam as it goes out the exit die, due to the drop of pressure, this results in a foam-like structure [36]. While reducing the feed moisture content can lead to increased expansion during processing [50], very high moistures (approximately 45%) combined with high protein ingredients like gluten can result in very dense products due to a smaller pressure differential. This effect can be desirable when producing meat analogous products, where the target is a dense and fibrous structure [48].

The composition of raw materials also has an effect on expansion index and bulk density. Protein is a main factor influencing these properties, as it has been reported that protein content reduces expansion ratio [51, 52]. Soy proteins have the capacity to work as an emulsifier between hydrophobic and hydrophilic materials, leading to smaller uniform air pockets in extrudates, increasing the bulk density [53]. Furthermore, the high temperatures of the extrusion process cause the denaturation of proteins, which can interfere with the proper swelling of starch granules as it makes starch and protein chains to "compete" for the available water [54].

4.1.3. Hardness

Hardness is an important sensory indicator corresponding to chewiness and mouthfeel. Hardness is positively correlated to feed moisture and heavily influenced by the expansion and bulk density of the extrudate. High moisture content reduces expansion, initially increasing hardness, whereas lower moisture content increases shearing action, reducing hardness. This occurs because higher screw speeds promote the gelatinization of starch, which improves texture by creating a uniform, fluffed-up consistency with reduced hardness and enhanced palatability (crispiness).

Increasing the feed moisture content tends to increase the breaking strength of the extrudates. However, very high moisture levels can result in an extrudate with a less dense internal structure, as moisture acts as a lubricant, reducing friction and adhesion between materials. As a result, extrudates with higher moisture content tend to exhibit lower hardness, tensile strength, and chewiness [55]. The viscoelasticity of gluten increases with rising extrusion temperatures; however, excessively high temperatures can cause protein denaturation and network rupture, which negatively affect gluten's viscoelasticity [40].

4.1.4. Digestibility

Extrusion enhances digestibility by altering the physical and chemical structure of the product through starch gelatinization and protein denaturation, as well as the destruction of antinutritional factors such as phytates, tannins, and trypsin inhibitors present in protein rich sources [56]. The shear forces of the extrusion process can partially break down the cellulose of high fiber ingredients like wheat, facilitating the release of the starch and protein contents, resulting in improved water retention and in vitro digestibility, as well as the reduction in size of the fiber chains, which increases bioavailability. This degradation of starch and proteins depends on the temperature and moisture content, Guldiken et al. [51] reported lower digestibility of chickpea and barley extrudates due to the high moisture content despite applying a high temperature profile along the extruder barrel. This was attributed to the source of protein also having an effect, they discussed the extrusion process cause an unfolding

of proteins in chickpea, improving digestibility, while reducing that of barley due to stronger denaturation, aggregation and formation of disulfide bonds.

5. TRADITIONAL OPTIMIZATION STRATEGIES: RESPONSE SURFACE METHODOLOGY AND ITS LIMITATIONS

Response surface methodology (RSM) has played a central role in food process optimization because it combines experimental design, regression analysis and graphical interpretation to identify operating regions associated with desirable product performance. Its value lies in its relative simplicity, its compatibility with central composite and Box-Behnken designs, and its capacity to provide interpretable polynomial equations linking process variables to quality responses. In extrusion studies, RSM has been used to optimize physical and functional responses such as expansion index, hardness, water absorption index and water solubility index, as well as nutritional and antioxidant attributes in products enriched with by-products such as mango peel, mango kernel, fruit residues and cereal co-products [57-59].

Despite these advantages, RSM is fundamentally constrained by the mathematical form it assumes. Most applications rely on second-order polynomial models, which are often adequate for smooth and moderately curved response surfaces but may fail when the system contains thresholds, asymmetrical effects, sharp transitions, or interactions that change across the experimental domain. Recent extrusion literature explicitly notes that, in high-moisture or structurally complex systems, traditional RSM can require many trials while still offering limited predictive power because it must force highly nonlinear behavior into a predefined polynomial form. For this reason, RSM remains useful for structured experimentation and first-pass interpretation, but it becomes less robust when the process space is heterogeneous, multivariable and strongly nonlinear [6].

In this sense, RSM should not be dismissed as an obsolete method, but rather repositioned as a valuable component within a broader modeling strategy. Its greatest strength lies in the generation of well-structured experimental datasets and in the identification of statistically meaningful trends during early-stage process development.

For researchers, RSM often provides an accessible starting point for screening variables, narrowing feasible operating regions and detecting first-order and curvature effects before more sophisticated algorithms are deployed. This makes it especially relevant when experimental budgets, raw material availability or pilot-plant access is limited. At the same time, the limitations of RSM become more evident as extrusion systems move away from conventional starch-rich formulations and toward multi-component matrices enriched with protein concentrates, lignocellulosic residues, oilseed cakes, fruit pomaces, or fermentation co-products. In such systems, the combined influence of composition and processing conditions may produce response patterns that are locally structured but globally irregular. Under these circumstances, RSM remains useful as a design-of-experiments framework, yet its predictive surface may oversimplify the process reality. Therefore, a more modern interpretation is to view RSM not as a final optimization solution, but as a foundational tool that can support subsequent machine learning development by generating informative, balanced, and experimentally datasets.

6. THE COMPLEXITY OF NONLINEAR INTERACTIONS: UNDERSTANDING THE “BLACK BOX” OF EXTRUSION

The notion of extrusion as a “black box” does not imply that the process is unknowable; rather, it reflects the fact that multiple transformations occur simultaneously and influence one another in ways that are difficult to isolate experimentally. Product quality and process efficiency depend not only on formulation composition, but also on extruder configuration, thermal profile, screw speed, moisture, hydration state, residence time, pressure development and specific mechanical energy. Reviews focused on aqua feed and pet food extrusion emphasize that feed formulation, machine configuration and operating conditions act together to determine texture, digestibility and nutritional value, while snack extrusion reviews similarly show that temperature and moisture strongly affect expansion, hardness and solubility-related properties [60, 61]. Another reason extrusion is frequently described as a “black box” is that many of its most important intermediate phenomena are not directly observable in real time. Structural transformations such as starch gelatinization, protein denaturation,

macromolecular alignment, partial depolymerization, melt formation and fiber disruption occur under coupled thermal and mechanical stresses inside the barrel, where direct measurement is difficult. As a result, researchers often infer internal process behavior indirectly through final product attributes or external process signals, such as die pressure, motor torque, specific mechanical energy and moisture loss. This indirect observation creates an interpretive gap between what happens inside the extruder and what can be measured outside it.

This complexity is further amplified when unconventional ingredients and agro-industrial by-products are incorporated. By-products vary widely in protein, fiber, starch, lipid, ash, particle size, hydration capacity and functional behavior, which alters the rheology of the feed blend and, consequently, the way heat and shear are translated into structure. Reviews on by-product extrusion underline that understanding these raw-material differences is essential because they directly modify both blend behavior before extrusion and product properties after extrusion. Under these conditions, similar changes in temperature or moisture may produce very different responses depending on ingredient composition, making the system difficult to represent through a single global quadratic equation [60, 62]. Unlike refined ingredients, by-products are inherently heterogeneous and may vary not only between sources, but also between harvest seasons, processing plants, particle-size distributions, and stabilization methods. Consequently, extrusion behavior is influenced not only by nominal ingredient identity, but also by hidden variability in material history and physicochemical functionality. From a modeling perspective, this means that the challenge is not simply to predict outputs from inputs, but to capture a system in which the effective behavior of the inputs may itself change from batch to batch. This is precisely why nonlinear, data-driven approaches are becoming increasingly attractive in extrusion science.

7. MACHINE LEARNING MODELS: ARTIFICIAL NEURAL NETWORKS AND ENSEMBLE METHODS

Machine learning (ML) addresses this challenge by shifting the focus from prespecified equations to data-driven pattern learning. Among the available approaches, artificial neural networks (ANNs) have been especially attractive in food process modeling because they can approximate complex nonlinear mappings between multiple inputs

and outputs. In extrusion, this means that ANN models can learn how formulation variables and machine settings jointly affect responses such as expansion, bulk density, firmness, water absorption and solubility.

Recent extrusion studies support the use of ML as a more flexible modeling framework than classical response surface approaches. For example, ANN-GA models have been shown to outperform RSM in predicting multiple extrusion responses in fortified plant-based extrudates, while newer studies in high-moisture protein extrusion report that machine learning-based optimization can converge with fewer experiments and lower prediction error than RSM. ANN, random forest, and XGBoost outperform classical polynomial models when predicting nonlinear extrusion responses. Beyond ANN, ensemble methods provide another important family of tools. Random forest builds a large collection of randomized trees and combines them to improve generalization; Breiman's original formulation also emphasized internal error estimates and variable-importance assessment, features that are highly useful when trying to identify the dominant processing factors in complex systems. XGBoost, in turn, represents a scalable implementation of tree boosting that has become widely used because of its strong predictive performance in tabular datasets and its ability to model nonlinear interactions efficiently. In a recent extrusion study using hemp residues as a sustainable ruminant feed ingredient, ANN, Random Forest, KNN, and XGBoost all outperformed quadratic regression across several responses, with the best-performing model depending on the target variable: XGBoost performed best for expansion index and bulk density, while ANN and Random Forest were particularly strong for water-related indices [4, 6, 63-65].

Instead of only explaining why a given formulation behaved in a certain way, ML models can estimate how a new formulation is likely to behave before it is physically tested, provided that it remains within a scientifically meaningful domain. This capability is especially useful in sustainable extrusion research, where the number of potential ingredient combinations can rapidly exceed what is practical to evaluate experimentally. By learning from prior trials, ML can help prioritize the most promising formulations and operating windows, thereby reducing time, cost, and material waste.

Nevertheless, predictive accuracy alone is not sufficient for scientific or industrial adoption. Model credibility depends on transparent validation, robustness across datasets and a clear understanding of the boundaries within which predictions remain reliable. In practice, this means that ANN, Random Forest, or XGBoost should be interpreted not as universal replacements for process knowledge, but as complementary tools whose usefulness depends on data representativeness, feature engineering and proper validation protocols. For extrusion applications, this balance between predictive power and scientific interpretability is particularly important, because models are expected not only to fit data, but also to support real decisions about formulation design, process adjustment, and quality assurance.

8. COMPARATIVE PERFORMANCE: WHY ML OFTEN OUTPERFORMS CLASSICAL MODELS

The main reason ML often surpasses classical regression in extrusion is not simply computational sophistication, but structural flexibility. Classical RSM is typically limited to main effects, pairwise interactions and quadratic curvature. By contrast, ML models can capture irregular response landscapes, hidden interactions and non-monotonic behaviors without forcing the system into a restricted polynomial architecture. This matters especially in extrusion, where the effect of one variable often depends on the value of several others at the same time. For example, the influence of screw speed may change depending on formulation moisture, fiber level, or protein source, and these dependencies may not be symmetric or linear across the design space. Broader food-processing reviews reach similar conclusions, noting that conventional experimental or mechanistic approaches often face extrapolation and modeling constraints, whereas ML offers stronger nonlinear fitting capacity for multifactor systems [66].

9. DATA SCIENCE AS AN ENABLING TOOL: FROM RAW DATA TO ACTIONABLE PROCESS INSIGHT

The real contribution of data science is not limited to generating better predictions; it lies in transforming dispersed experimental observations into actionable process knowledge. In extrusion research, this requires a structured workflow: selection of

relevant inputs, consistent data logging, preprocessing, model training, validation and interpretation. A recent extrusion ML study explicitly incorporated outlier detection, winsorization, normalization, hyperparameter tuning, cross-validation and independent external validation before comparing models. This is a crucial point: predictive performance in food processing is not only a function of the algorithm chosen, but also of data quality, preprocessing rigor and the way training and testing sets are defined [63].

More broadly, recent reviews of machine learning in food processing and food quality control argue that the next step is not simply to accumulate more models, but to integrate ML into intelligent, transparent and scalable processing systems. Key challenges include small datasets, overfitting risk, limited interpretability, legacy-system integration and the need for explainable industry-ready tools. Therefore, in the context of sustainable extrusion, data science should be viewed as an enabling framework that links ingredient characterization, process optimization, quality prediction and eventually digital process control. In practical terms, this means moving from isolated experimental datasets toward interoperable databases, hybrid mechanistic-ML strategies, feature-importance analysis and real-time monitoring architectures aligned with Industry 4.0 principles [66, 67].

A key implication of this perspective is that successful data science in extrusion begins long before model training. It starts with experimental discipline: standardized raw-material characterization, traceable batch identification, calibration of sensors, harmonized response measurements and rigorous metadata collection. Without these elements, even advanced algorithms may learn patterns that are unstable, biased or non-transferable. Therefore, the digitalization of extrusion should be understood as both a computational and an experimental challenge, requiring close integration between process engineering, ingredient science, statistics and informatics. In the longer term, this opens the possibility of developing intelligent extrusion platforms capable of supporting adaptive process management. Such systems could combine ingredient databases, historical production records, inline sensor signals and predictive models to assist with formulation adjustment, anomaly detection and quality forecasting.

Although full real-time optimization remains an emerging goal, the conceptual pathway is already clear: from isolated experiments to curated datasets, to validated predictive models and finally to decision-support systems embedded within industrial practice. Within this framework, data science becomes more than an analytical tool; it becomes an infrastructural element for building sustainable, resilient and knowledge-driven extrusion systems aligned with circular bioeconomy objectives.

10. THE DATA-DRIVEN DESIGN FRAMEWORK: A STRUCTURED ROADMAP

The shift toward "intelligent" extrusion is a fundamental evolution in food and feed engineering, moving away from legacy "trial and error" methods toward a disciplined, predictive environment. Rather than viewing the extruder as a series of isolated batches, this modern approach treats the process as an integrated system [68]. To bridge the gap between variable raw ingredients and optimized final products, the industry must adopt a framework built upon five critical pillars.

The foundation of this system is *Comprehensive Ingredient Characterization*. It is no longer affordable to view agro-industrial by-products as simple bulk fillers defined by weight. Instead, a high-resolution chemical and physical audit is required to quantify nuances like fiber morphology and protein solubility [6]. For instance, when utilizing residues like hemp, understanding the specific rheological properties—how these fibers influence the flow of the melt—is essential for creating an accurate initial data layer [69].

Building upon this data, *Robust Experimental Design* ensures that machine learning models are trained on high-quality information that captures the "edges" of the process. This needs to move away from changing one variable at a time in favor of structured designs that highlight how formulation changes interact with mechanical energy and thermal profiles [70]. By intentionally exploring these interactions, diverse datasets needed for algorithms are created to learn the true physics of the barrel.

Because raw extrusion data is inherently noisy and often nonlinear, *Intelligent Data Preprocessing* is a vital third step. This phase involves cleaning and normalizing the data to ensure that algorithms, such as artificial neural networks, are learning from true

physical signals rather than experimental artifacts or sensor interference [71]. Standardizing data in this way also allows the resulting tools to remain scale-agnostic, facilitating the jump from lab-scale research to industrial production.

The utility of these models is ultimately confirmed through *Iterative Model Validation*. A predictive tool is only as good as its performance against unknown variables, so these tools must be tested against real-world pilot runs. By seeking a high correlation between predicted metrics, such as expansion or density, and the actual physical results coming out of the die, the improved predictive performance of a data-driven approach can be verified [72].

Finally, the framework culminates in *Multi-Objective Optimization*. Industrial production is rarely about hitting a single goal; it is a delicate balancing act between functional excellence, nutritional integrity, and resource efficiency. By utilizing the predictive power of machine learning to map the "Pareto frontier," engineers can find the mathematical "sweet spot" where the use of sustainable by-products is maximized without compromising the structural stability, nutritional quality or sensory properties of the product [73]. This approach ensures that technical success is perfectly aligned with the broader principles of a circular bioeconomy.

11. IMPLEMENTATION LIFECYCLE: TRANSLATING DATA INTO PRODUCTION

The transition of a data-driven model from the controlled environment of a research laboratory to a fully functional production line is a complex journey that demands a rigorous, multi-stage lifecycle. This process is essential to ensure that the theoretical frameworks designed for "intelligent" extrusion actually yield high-quality and sustainable results when applied to real-world manufacturing [74]. The journey begins with *High-Resolution Ingredient Characterization*, a phase that goes far beyond the surface-level information found on standard nutritional labels. When working with agro-industrial by-products like hemp or other fiber-rich residues, a deep chemical and physical inspection is mandatory [17]. This involves quantifying rheological properties to understand exactly how these specific fibers influence the flow of the melt within the barrel [35] or evaluating the chemical composition of agro-industrial by-products [61].

By mapping the natural composition variance inherent in sustainable by-products, researchers can better prepare their models for the inevitable fluctuations in raw material input [75].

Once the materials are characterized, the focus shifts to *Strategic Data Preprocessing and Curation*. Extrusion data is notoriously complex, often characterized by nonlinear relationships and mechanical noise from the machinery itself. To find the true physical signal of the process, rigorous noise reduction is required to filter out sensor interference [76]. Furthermore, data normalization ensures that the machine learning tools remain "scale-agnostic," allowing insights gained on a pilot plant scale to be accurately translated to industrial-level equipment [77].

The third stage, *Model Training and Blind Validation*, utilizes advanced computational tools like artificial neural networks or ensemble methods to "learn" the intricate interactions between formulation changes and processing parameters [78]. To ensure the system's reliability, it is subjected to strict validation protocols where it must predict functional properties—such as expansion and bulk density—for experimental datasets it has never encountered before [79]. This cross-verification against traditional empirical results is critical for demonstrating that the data-driven approach offers a significant improvement in predictive performance over legacy methods [80].

The lifecycle concludes with *Real-Time Deployment and Multi-Objective Tuning*. This involves integrating the validated model directly into the factory's control system to create an intelligent feedback loop. As the extruder operates, real-time data is continuously fed back into the model to refine its accuracy, creating a self-improving system that learns on the job [81]. This allows for constant optimization alignment, where machine parameters are adjusted in real-time to hit the "sweet spot" where technical product quality meets the ambitious sustainability goals of a circular bioeconomy [31].

12. MULTI-OBJECTIVE OPTIMIZATION: BALANCING TECHNICAL PERFORMANCE WITH CIRCULAR GOALS

In the final stage of this methodology, the focus shifts from simply ensuring a process "works" to ensuring it operates optimally across a spectrum of competing priorities. This is

the critical juncture where the theoretical framework encounters the complex reality of industrial production, demanding a delicate balance between engineering precision and environmental responsibility [82]. Unlike traditional extrusion, which often pursued the singular goal of maximizing throughput or achieving a specific texture, a sustainable, data-driven approach requires the simultaneous optimization of multiple outcomes.

Achieving *Functional Excellence* remains a primary objective, as the product must meet rigorous physical standards, including specific expansion ratios, bulk density, and solubility to ensure consumer or industrial acceptance [83]. However, this must be balanced with *Nutritional Integrity*. The high-shear environment within an extruder barrel can be detrimental to heat-sensitive proteins and vitamins; thus, the process must be tuned to protect these vital components while still achieving the desired physical structure [84].

At the heart of the circular bioeconomy is *Maximized Valorization*, which involves pushing the inclusion levels of agro-industrial by-products as high as possible. This is often a technical challenge, as these materials can interfere with the structural stability of the final extrudate [58]. Furthermore, *Resource Efficiency* must be integrated into the control logic to reduce energy consumption and minimize waste during the high-variability phases of startup and production transitions [85].

Finding the "sweet spot" among these objectives is difficult because they are frequently in conflict—for instance, increasing fiber content for higher valorization typically has a negative impact on product expansion [59]. To navigate these trade-offs, the predictive power of machine learning is used, such as ensemble methods, to map the "Pareto frontier" [66]. This mathematical space identifies the limits of performance where one objective cannot be improved without degrading another. By visualizing these complex relationships, researchers and engineers can make informed, data-backed decisions that align with the core principles of a circular bioeconomy [31]. Ultimately, this approach ensures that the resulting food or feed is not just a technical success but a sustainable one that actively contributes to waste reduction and resource efficiency [86].

13. SUSTAINABILITY AND CIRCULARITY: ASSESSING ENVIRONMENTAL IMPACT AND WASTE VALORIZATION

This final phase of the implementation marks a strategic transition from technical execution to a holistic evaluation of the process through the lens of the circular bioeconomy. The primary goal is no longer just machine efficiency but quantifying the "green" impact that an intelligent extrusion framework delivers to the global food system [6]. By moving away from resource-heavy conventional ingredients and adopting a data-driven approach to upcycling, it can be ensured that industrial production stays within boundaries.

A cornerstone of this evaluation is the *Environmental Footprint Assessment*, since it analyzes the broader implications of replacing traditional animal proteins or refined starches with agro-industrial by-products like hemp residues [63]. This assessment is vital because it moves beyond simple carbon counting to look at the entire lifecycle of the material. In this context, extrusion is positioned as a key enabling technology, a "waste valorization" engine that transforms underutilized, low-value materials into functional, stable, and nutritionally dense products [58].

The framework also prioritizes *Resource Efficiency* by aligning predictive modeling with circular principles. By utilizing machine learning to "get it right the first time," it can drastically reduce the energy consumption and material waste typically associated with the lengthy trial-and-error phases of traditional optimization [62]. Finally, through *Bioeconomy Integration*, the framework ensures that ingredient development isn't just a technical achievement but is strategically synchronized with global sustainability goals. This ensures that every kilogram of upcycled material contributes to a more resilient, resource-efficient food system that actively reduces waste rather than merely managing it [55].

14. THE FUTURE OF EXTRUSION: INTELLIGENT CONTROL SYSTEMS AND EMERGING RESEARCH

The final section of this chapter pivots toward the next frontier of food and feed engineering: the transition from static, offline models to autonomous, real-time systems. While moving beyond the laboratory, the focus shifts to how these "intelligent"

frameworks can be embedded directly into the industrial landscape to create a more responsive and resilient production environment.

The cornerstone of this evolution is the development of *Intelligent Control Systems*. By integrating machine learning algorithms—such as artificial neural networks and ensemble methods—directly into the extruder's hardware, it moves toward real-time process adjustments [71]. Unlike traditional systems that rely on periodic manual sampling and reactive troubleshooting, these intelligent setups utilize "soft sensors" to infer internal melt properties, such as viscosity and molecular degradation, as they happen [53]. This allows the machinery to maintain consistent product quality even when faced with the inherent variability of upcycled ingredients.

Looking further ahead, research is increasingly focused on "Closing the Loop". The goal is to develop "self-correcting" extruders equipped with advanced in-line spectroscopic sensors, such as Near-Infrared (NIR) or Raman probes [66]. These systems can sense minute fluctuations in raw by-product quality—such as shifts in fiber morphology or protein solubility—and instantly adjust heat, moisture, or shear levels to compensate [67]. This level of autonomy is essential for the commercial viability of a circular bioeconomy, as it prevents large-scale material waste during ingredient transitions.

This *Data-Informed Evolution* represents a permanent shift in the industry, moving away from empirical, "black-box" process control toward fully predictive and transparent optimization. By bridging experimental research with these emerging computational methods, a unified path is provided for researchers and industry professionals to lead the transition to a more resilient food system. Ultimately, these smart systems ensure that high-quality nutrition can be produced sustainably at a global scale, aligning technical excellence with the urgent demands of resource efficiency.

Conclusions

Extrusion provides an effective technological platform for converting agro-industrial by-products into functional food and feed ingredients, thereby creating opportunities to improve resource utilization and support circular bioeconomy strategies. Nevertheless, the incorporation of heterogeneous materials such as cereal bran, fruit pomaces,

oilseed cakes and meals, and other fiber- or protein-rich residues increases the complexity of an already highly interactive process. Their variable composition affects rheology, heat and mass transfer, mechanical energy dissipation, and ultimately the nutritional, structural, and functional properties of the extrudate. Consequently, successful valorization cannot rely solely on increasing by-product inclusion but requires careful integration of ingredient characteristics with processing conditions and desired product attributes.

Traditional approaches such as response surface methodology remain valuable for experimental design, variable screening, and the identification of general process trends. However, their predefined polynomial structure can limit their ability to represent the nonlinear and conditional interactions characteristic of complex extrusion systems. Machine learning approaches, including artificial neural networks and ensemble methods, together with Bayesian and multi-objective optimization, provide complementary tools capable of learning more complex relationships among formulation variables, operating conditions, and product responses. Their value is particularly relevant when several competing objectives must be considered simultaneously, including product structure, nutritional quality, process stability, resource efficiency, and maximum incorporation of sustainable raw materials.

The transition toward data-driven extrusion, however, depends on more than algorithm selection. Reliable ingredient characterization, structured experimental design, rigorous preprocessing, representative datasets, independent model validation, and appropriate interpretation are essential for developing models that can be transferred beyond the conditions under which they were trained. Future progress should therefore emphasize standardized and interoperable datasets, hybrid approaches combining mechanistic knowledge with machine learning, explainable models, and integration with inline sensing and real-time monitoring.

Ultimately, the convergence of extrusion engineering, ingredient science, and data science provides a pathway from empirical trial-and-error optimization toward predictive and adaptive manufacturing. Intelligent control systems capable of responding to variations in raw-material properties could improve product consistency

while reducing experimental trials, material losses, and resource consumption. Such developments will be particularly important for the large-scale valorization of variable agro-industrial by-products, positioning data-driven extrusion as an enabling technology for more resilient, resource-efficient, and sustainable food and feed production.

Conflict of Interest statement

The authors declare no conflict of interest.

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The authors have no specific acknowledgements to declare.

Author's Contribution

Jorge Iñaki Gamero-Barraza contributed primarily to the development of Part 1, including sustainable raw-material selection, specialized extrusion applications, physicochemical transformations, and functional properties of extruded products. Aylin Socorro Saenz-Santillano contributed primarily to Part 2, focusing on traditional optimization strategies, nonlinear interactions in extrusion processes, machine-learning models, comparative predictive performance, and data-science approaches. Damián Reyes-Jáquez contributed primarily to Part 3, developing and integrating the data-driven design framework, implementation strategies, multi-objective optimization, sustainability and circularity considerations, and future perspectives on intelligent extrusion systems. Efren Delgado and Cristian Patricia Cabrales-Arellano contributed to the conceptual development of the chapter, scientific discussion, critical review, and refinement of the manuscript. Damián Reyes-Jáquez coordinated the overall structure and integration of the chapter. All authors reviewed and approved the final manuscript.

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