AI-Based Surrogate Models for the Food and Drink Manufacturing Industry: A Comprehensive Review

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Citation:

LWELE, Emmanuel, SHENFIELD, Alex and DA SILVA, Carlos Eduardo (2025). AI-Based Surrogate Models for the Food and Drink Manufacturing Industry: A Comprehensive Review. Processes, 13 (9): 2929. [Article] processes

Review

AI-Based Surrogate Models for the Food and Drink Manufacturing Industry: A Comprehensive Review

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Abstract

Surrogate models provide virtual representations that mirror physical objects or processes, serving distinct purposes in simulations and digital transformation. This review article examines how integrating surrogate modelling with artificial intelligence (AI) techniques can facilitate the iterative development of surrogate models and identify instances where additional data acquisition is necessary to enhance the performance of a surrogate model. This demonstrates the potential of combining AI with surrogate modelling in addressing some of the key challenges in the food and drink manufacturing industry. The paper also provides an accessible examination of AI and surrogate modelling in the food and drink manufacturing industry, offering a summary of current applications and advancements within the field. The key areas addressed by this article include the application of AI and ML in process control, prediction, and modelling for food manufacturing, as well as the advantages and limitations of AI-based surrogate modelling (SM), among other issues addressed. Based on the literature reviewed herein, AI-based surrogate models can be employed to optimise production processes and reduce the need for extensive physical prototyping in the food and drink manufacturing industry. This review emphasises AI-based surrogate modelling techniques tailored for complex food processing systems and distinguishes itself by bridging method-specific insights with practical industrial relevance. Additionally, this article reviews challenges and limitations in the food and drink manufacturing industry and the application of surrogate modelling, along with future directions for research in this rapidly evolving field.

Keywords: surrogate models (SMs); artificial intelligence (AI); food manufacturing; process optimisation; digital twins; predictive maintenance; machine learning (ML); sustainability; data-driven modelling; industrial applications

Academic Editor: Claudio Urrea

Received: 3 July 2025
Revised: 8 September 2025
Accepted: 11 September 2025
Published: 13 September 2025

Citation: Lwele, E.; Shenfield, A.; da Silva, C.E. AI-Based Surrogate Models for the Food and Drink Manufacturing Industry: A Comprehensive Review. *Processes* **2025**, *13*, 2929. https://doi.org/10.3390/pr13092929

1. Introduction

During the past decade, the integration of artificial intelligence (AI) into the food and drink manufacturing industry has expanded rapidly, driven by technological progress, advances in data availability, processing power, and machine learning (ML) techniques, and the growing need for improved efficiency and productivity [1]. According to [2], adopting AI, particularly through AI-based surrogate models, has been shown to positively influence internal environmental management, ecodesign and corporate asset management, while also optimising production processes, reducing prototyping costs, and improving product quality, ultimately advancing sustainability in the food and drink manufacturing industry. The integration of AI in the food and drink manufacturing industry is also linked to the promotion of circular economy practices.

Recent syntheses highlight how AI is simultaneously reshaping personalised nutrition (PN) and intelligent food manufacturing, with shared methods such as multi-omics modelling, computer vision, and federated learning (FL) for privacy-preserving analytics. The reviews emphasise digital twins for virtual experimentation and process optimisation, and call for explainable models to support regulatory acceptance and equitable deployment across populations [3].

This review focuses specifically on AI-based surrogate modelling within the food and drink manufacturing context. While previous reviews have addressed AI applications broadly, such as the application of artificial intelligence and big data in the food industry [4] or machine learning in food quality determination, control tools, classification, and prediction [5], this article offers a focused synthesis of the technical methodologies and industrial relevance of AI-based surrogate models in the food and drink manufacturing sector. The novelty lies in bridging recent developments in AI with surrogate modelling applications unique to food systems.

Canatan et al. (2025) provide a broad review article in *Food Engineering Reviews* on AI in food manufacturing, covering machine learning, computer vision, robotics, and NLP across quality control, predictive maintenance, and safety [6]. Although comprehensive in application breadth, the paper does not deeply examine surrogate modelling as a methodological pillar for digital twins or physics-informed surrogates for regulatory-grade process understanding. In contrast, our review unifies AI-based surrogate modelling with digital twin design for food and drink manufacturing, detailing how PINNs and AI-based surrogate models can be deployed as surrogates, alongside design of experiments and multifidelity data strategies.

Food processing often includes complexities and dynamic difficulties that make direct simulation impractical and very costly. Surrogate models thus not only reduce computational effort but also offer a pathway to emulate systems where first-principles models are infeasible.

A study by Graetz and Michaels [7], indicated that AI-powered robots contributed to a quarter of GDP growth in several countries from 1993 to 2007, suggesting a significant role for AI in improving productivity [2].

AI-based surrogate models are significantly transforming various industries by enhancing efficiency, reducing costs, and accelerating innovation. Section 3 will provide a detailed definition of surrogate modelling and a generic framework for developing surrogate models, highlighting their purpose and workflow in computational modelling processes. For example, in the field of material design, AI-based surrogate models have contributed to the rapid development of bio-inspired materials and the optimisation of mechanical properties, significantly shortening the time required to bring new materials to market [8]. Surrogate models can also be utilised for design optimisation and performance prediction of complex systems, such as in the aerospace and automotive industries, simulating aerodynamic properties or structural integrity under various conditions, allowing engineers to make informed decisions without the need for exhaustive testing [9,10]. Surrogate models can leverage historical data and predictive analytics to support organisations in making informed decisions regarding material selection, process optimisation, and product development, leading to improved outcomes and competitive advantages [8].

AI-based surrogate models can potentially transform industries by providing faster, more effective, and cheaper process modelling. The ability of surrogate models to estimate results and predict design improvements is a powerful resource for addressing complex issues and improving efficiency in the food and drink industry and other sectors, which were not easily achievable in the past. This capability is changing the face of the food and drink industry, engineering, and other fields.

This paper comprehensively reviews AI-based surrogate modelling and its growing significance in the food and drink manufacturing industry. Section 2 introduces the methodology used in this review, highlighting the inclusion and exclusion criteria of articles and the databases used in conducting this review. Section 3 delves into the fundamental principles, highlighting the definition, purpose, and structured workflow of surrogate modelling. In Section 4, this paper shifts towards AI-driven approaches, offering insights into machine learning fundamentals and specialised techniques tailored for surrogate modelling. Section 5 provides a detailed exploration of state-of-the-art techniques, including physics-informed neural networks (PINNs), convolutional neural networks (CNNs), and recurrent neural networks (RNNs), alongside their practical applications in the food and drink manufacturing industry. Section 6 examines the transformative impact of surrogate models within the food and drink industry, emphasising their role in process optimisation and energy efficiency. Section 7 assesses the prevailing challenges and limitations within the field, leading into Section 8, which explores future research directions in the application of surrogate modelling in the food and drink manufacturing industry. This emphasises the importance of addressing the outlined challenges to maximise the potential of artificial intelligence (AI) and surrogate models (SMs) in reducing the cost of extensive physical prototyping.

2. Methodology

A structured literature review methodology was adopted in this study to ensure a comprehensive, transparent, and reproducible synthesis of current research. While this methodology is not fully systematic, it draws from systematic review principles outlined by Anlesinya et al. [11].

2.1. Data Sources

The primary sources included Scopus, Google Scholar, and IEEE Xplore, which were selected due to their extensive coverage of high-quality peer-reviewed research in food engineering, artificial intelligence, and industrial applications. These databases were queried using relevant keywords associated with surrogate models and their applications in the food and drink manufacturing industry.

2.2. Search Strategy

The search strategy employed a combination of Boolean operators and controlled vocabulary, which was developed iteratively following a preliminary scan of the literature. Keywords were chosen to reflect the intersection of surrogate modelling, AI techniques, and food and drink manufacturing.

This review focused on publications released between 1 January 2014 and 1 April 2025 to capture the most recent advancements in the field. Studies included in this review encompassed peer-reviewed journal articles, conference proceedings, technical reports, and high-impact reviews that specifically discuss the role and development of surrogate models within the industry. Articles were screened based on their relevance, with an emphasis on works that provided empirical evidence, case studies, or theoretical advancements related to surrogate modelling.

Beyond synthesising current research, this review identifies several promising avenues for future studies in the application of surrogate models within the food and drink manufacturing industry. It also provides recommendations for expanding the practical adoption of surrogate modelling techniques, addressing existing limitations, and exploring emerging trends in artificial intelligence-driven process optimisation.

3. Surrogate Modelling

This section provides a detailed overview of surrogate modelling, its definition, purpose, and associated framework. Section 3.1 discusses the fundamental concepts of surrogate modelling; Section 3.2 outlines the surrogate modelling framework and workflow, detailing the step-by-step procedure for constructing a surrogate model and illustrating the workflow, from design parameters and simulation data to the training and application of surrogate models in various industrial tasks.

3.1. Definition and Purpose of Surrogate Modelling

Surrogate modelling is a computational technique used to create simplified models that approximate the behaviour of complex, computationally expensive simulations or physical processes. Figure 1 illustrates the workflow of using surrogate models to approximate expensive simulations in computational processes. The design parameters, denoted as $X_1, X_2, \ldots, X_N$, are input into simulations to evaluate the actual function $y = f(X)$, which is often computationally expensive due to the need for multiple simulation runs. To reduce costs in simulations of computational processes, a surrogate model $\hat{f}(X)$ is fitted using a dataset of input–output pairs $(x^i, f(x^i))$. Once trained, the surrogate model will serve as a computationally inexpensive approximation of $f(X)$, enabling efficient sensitivity analysis, optimisation, and risk analysis. The red dashed arrows highlight the high computational cost of simulations, while the blue arrows indicate the cost-effectiveness of using surrogate models for analysis.

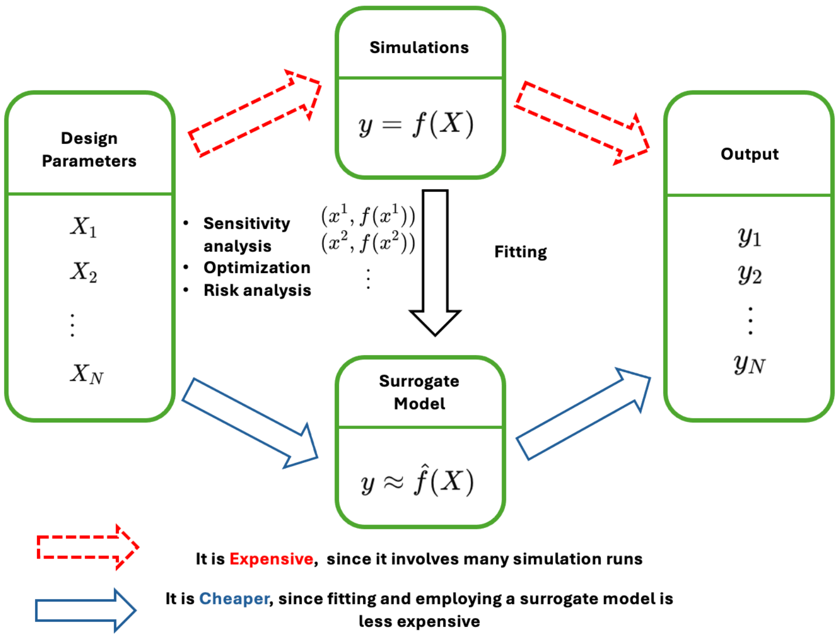

Figure 1. Overview of surrogate modelling process.

In this review, the term surrogate modelencompasses two complementary classes, as follows: (i) *Simulation-sourced (high-fidelity) surrogates*, which approximate outputs of a mechanistic model (e.g., PDE-based or CFD) that is computationally expensive to evaluate; and (ii) *Experiment-calibrated statistical/ML emulators*, which learn a predictive mapping directly from experimental or plant data to accelerate optimisation, reduce costly trials, or enable real-time decision support. Both classes serve the surrogate modelling objective of *fast*, *sufficiently accurate* prediction for design-space exploration, optimisation, control, or digital twins. In Sections 5 and 6, this review includes studies where the surrogate replaces either a computationally intensive mechanistic model or repeated physical experimentation, and annotates the context accordingly.

The primary goal of surrogate modelling is to reduce computational costs associated with tasks such as optimisation, sensitivity analysis, and uncertainty quantification [12]. Surrogate models are defined as computationally efficient approximations of more complex or costly models, including both purely data-driven mappings and reduced-order or hybrid mechanistic surrogates [13]. They are instrumental in scenarios where the original model is computationally expensive to evaluate multiple times, such as in optimisation problems or when conducting extensive simulations [14].

One of the primary advantages of surrogate models is their ability to optimise processes in scenarios where traditional models require extensive computational resources; surrogate models can be employed to explore the design space more efficiently. For instance, in optimising catalytic reforming and the isomerisation processes, surrogate models can replace detailed process simulations, allowing engineers to quickly evaluate multiple design alternatives without the need for time-consuming calculations [15]. Surrogate models are particularly valuable in situations where the original models are either too complex to be used directly or where computing the model derivatives is complex. For example, in the design of distillation columns, surrogate models based on Kriging interpolation can be utilised to approximate the performance of the columns without requiring direct access to the detailed simulation models. This capability of surrogates is essential in industrial settings where rapid decision-making is critical, and the ability to quickly assess the impact of design changes can lead to significant cost savings and improved operational efficiency [16]. In food and drink applications that require optimisation, surrogate models also play a vital role in sensitivity analysis and uncertainty quantification. Surrogate models thus enable engineers to assess how variations in input parameters affect system performance. This is particularly important in industries where processes are subject to uncertainties, such as fluctuations in feed composition or operating conditions. Surrogate models can help identify critical parameters that influence system behaviour, allowing for more informed decision-making and risk management [17]. Integrating surrogate models into digital twin frameworks enhances their applicability in real-time monitoring and control of industrial processes. Digital twins, which are virtual representations of physical systems, can leverage surrogate models to simulate and predict system behaviour under various operating conditions. Integrating surrogate models enables proactive adjustments in response to changing conditions, ultimately leading to improved process reliability and efficiency [14]. Surrogate models can help reduce computational costs while ensuring accuracy in the food and drink sector. In the future, the use of surrogate models is expected to grow, thus enhancing their application in the food process design and optimisation.

3.2. Surrogate Modelling Framework and Workflow

The workflow in Figure 2, illustrates the step-by-step procedure for building a surrogate model, followed by a paragraph of each step in the surrogate model workflow, each contributing to the development and validation of a surrogate model.

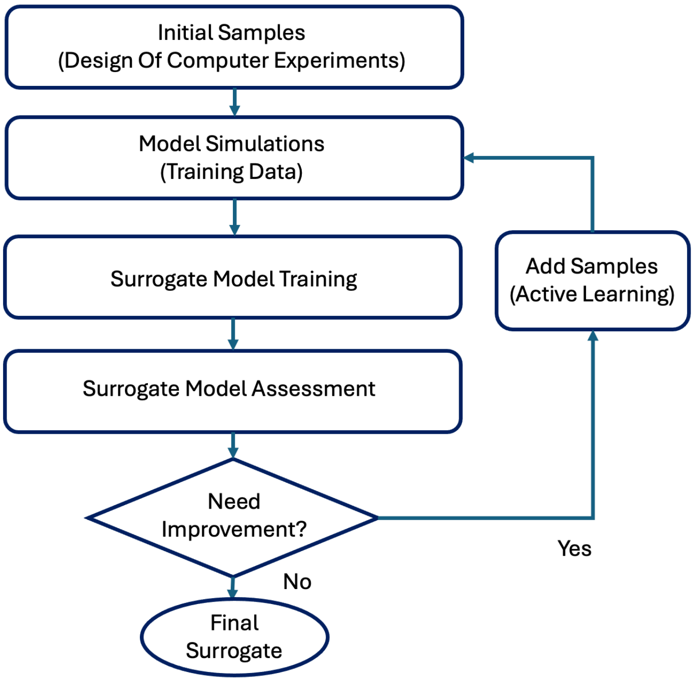

Figure 2. Data-driven surrogate modelling framework and workflow. This figure illustrates the step-by-step procedure for building a surrogate model.

The surrogate modelling framework and workflow are a systematic approach that enables the efficient approximation of complex models, particularly in scenarios where computational resources are limited. Below is a detailed description of each stage involved in the surrogate modelling workflow in Figure 2.

i. Initial Samples (Design of Computer Experiments):

The first stage in the surrogate modelling process is to generate an initial set of training data points or samples. This process is led by a DoE (design of experiments) approach to guarantee that the samples are well spaced throughout the input parameter space. The goal is to encompass a wide range of conditions that the system may encounter. Various sampling techniques can be employed, such as Latin hypercube sampling, factorial design, or random sampling, to create a representative training dataset. The quality and distribution of these initial samples are crucial, as they directly influence the accuracy and reliability of the surrogate model that will be constructed later [9,18].

ii. Output Evaluations (Training Data Generation):

After the initial samples are chosen, the following step is to compute these samples using a high-fidelity model, such as finite element analysis (FEA) or computational fluid dynamics (CFD). Every sample is fed into the high-fidelity model, and the output values are obtained for each sample in turn, resulting in a set of input–output data. This dataset forms the foundation for training the surrogate model. The accuracy of the surrogate model heavily relies on the quality of this training data, as it must effectively represent the underlying relationships between the input parameters and the output responses [19].

iii. Surrogate Model Construction:

The surrogate model is constructed using the training data obtained from output evaluations. Various machine learning techniques can be employed for this purpose, including polynomial regression, Gaussian processes, artificial neural networks, and radial basis functions [18]. The choice of the surrogate model depends on the complexity of the problem and the nature of the dataset. Surrogate models learn the relationship between inputs and outputs, creating a computationally inexpensive representation of the original complex model. This model can then be used to predict outputs for new input configurations without the need for extensive simulations [17].

iv. Surrogate Model Assessment:

After generating the surrogate model, it is essential to evaluate its performance and accuracy. This assessment is typically performed by comparing the surrogate model's output with the actual output of the high-fidelity model on a separate dataset that was not used in training the model. Some of the error metrics commonly used to determine a model's accuracy include mean squared error and R-squared values. If the surrogate model does not meet the desired accuracy criteria, it may require further refinement or retraining. This assessment stage is critical to ensure that the surrogate model is a reliable approximation of the actual process [19].

v. Iterative Improvement (Need for Additional Samples):

In many cases, the first surrogate model may not be sufficiently accurate for the specific task it is intended to support. This is the stage where it is established whether the model's performance is adequate for particular requirements. If the surrogate model is considered inadequate, more samples may be required to enhance the model's accuracy. This decision-making process is crucial, as it helps to identify whether further refinement is necessary or if the model can be utilised as is [19].

vi. Active Learning (Adding Samples):

If the surrogate model needs to be improved, then new samples can be taken using an active learning strategy. This method selects new sample points that are likely to be beneficial for the model in areas of the design space where the model yields poor results. The process of sampling and training is performed sequentially until the surrogate model achieves the desired level of accuracy. This approach helps in reducing the number of new simulations that are needed and, hence, reduces the computational costs that are incurred while trying to build the surrogate model that is both accurate and efficient [19]

vii. Final Surrogate Model:

When the surrogate model has reached the required level of precision, it is referred to as the final surrogate model. This model can then be used for various applications, including optimisation, quantification of uncertainty, sensitivity analysis, or real-time decision-making. The final surrogate provides a computationally efficient alternative to the original complex model, enabling faster evaluations and more effective analyses. The last surrogate is a less complex model, which is easier and quicker to evaluate and analyse as compared to the original model. This stage is the last step of the surrogate modelling process, and the model is now in a form that can be used in engineering and design [19]. The construction of the surrogate model relies on input data, and through active learning and iterative enrichment of the training dataset, the model is refined to achieve high accuracy and efficiency.

The workflow in Section 3.2 applies to both simulation-sourced and experiment-calibrated surrogates. In the case of *simulation-sourced surrogates*, the high-fidelity (HF) data stem from mechanistic simulations (e.g., FEM/CFD/PDE solvers), possibly at multiple fidelities. In the case of *experiment-calibrated surrogates*, training data arise from designed experiments or historical plant data. Physics-informed training (e.g., PINNs) is a *training paradigm* that can be applied atop common architectures (FNN/CNN/RNN/transformers) and is compatible with either branch, where governing equations or constraints are available.

4. AI-Based Approaches in Surrogate Modelling

Surrogate modelling is increasingly using artificial intelligence (AI), specifically machine learning (ML), techniques in its implementation. This shift is due to the growing complexity and computational expenses of more conventional modelling strategies. Within AI, ML is a specific field that focuses on algorithms that can learn from data. This data-driven approach provides a method for developing models that can utilise a small subset of the input data to potentially represent the remainder of the design space.

4.1. Introduction to Machine Learning

Machine Learning (ML) is a dynamic and rapidly evolving field within artificial intelligence (AI) that emphasises the development of algorithms and models that enable computers to learn from data and make predictions or decisions without being explicitly programmed for each specific task [20]. Machine learning can be defined as a subset of artificial intelligence that focuses on creating systems capable of learning from data. The primary goal of ML is to develop algorithms that can identify patterns within data and use these patterns to make predictions or decisions about new, unseen data. This learning process is often achieved through the analysis of large datasets, allowing the model to improve its performance over time as it encounters more data [21].

The concept of machine learning is not new; it has its roots in the early days of computing. Pioneers like Alan Turing and John McCarthy laid the groundwork for the field, with Turing discussing the potential for machines to learn from experience as early as 1950 [20]. The resurgence of interest in ML in recent years can be attributed to the exponential growth of data availability and computational power, as well as the development of more sophisticated learning algorithms [21].

4.1.1. Distinction Between Traditional Expert Systems and Machine Learning

The distinction between machine learning and traditional expert systems is significant. In conventional expert systems, a programmer writes explicit rules and instructions that dictate how a computer should perform a specific task as shown in Figure 3. This approach is often referred to as rule-based programming. For example, a rule-based system might include instructions such as "If the temperature exceeds 100 degrees, then activate the cooling system."

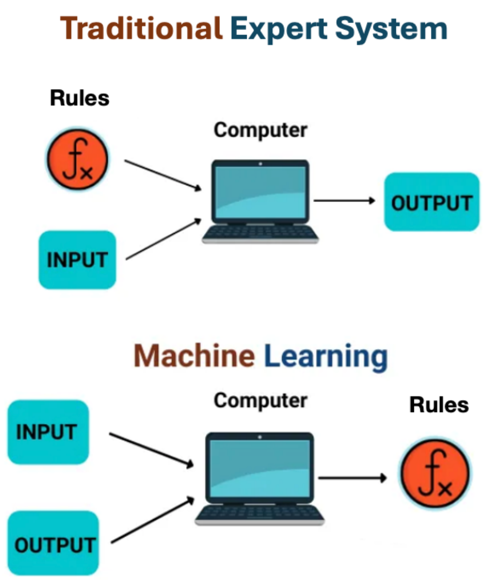

Figure 3. Comparison between traditional expert systems and machine learning.

In contrast, machine learning systems do not rely on predefined rules. Instead, they learn from examples. For instance, a machine learning model might be trained on historical data of temperature readings and cooling system activations. Through this training process, the model learns to recognise patterns and can make predictions about when to activate the cooling system based on new temperature data, even if it has never encountered that specific scenario before [9,22]. This fundamental difference allows machine learning systems to adapt to new information and improve their performance over time, making them particularly well-suited for tasks where the rules are complex or not well understood.

All machine learning algorithms consist of three main components: data, model, and loss function.

4.1.2. The Data

Data is the foundational element of any machine learning model. It can take various forms, including structured and unstructured data. The quality and quantity of the data significantly influence the performance of the machine learning model. For effective learning, the data must be representative of the problem domain and contain relevant features that enable the model to make accurate predictions [9,23].

4.1.3. The Model

The model is a mathematical representation of the relationships within the data. It is constructed using algorithms that process the input data to learn patterns. Different types of models can be used depending on the nature of the problem, such as regression models to predict continuous outcomes or classification models to categorise data into discrete classes. The choice of model is crucial, as it determines how well the system can learn from the data [20,22].

4.1.4. The Loss Function

The loss function is a component that quantifies how well the model's predictions align with the actual outcomes. It measures the difference between the predicted values and the true values, providing a metric for the model's performance. The goal of training a machine learning model is to minimise this loss function, thereby improving the accuracy of the predictions. The optimisation process of machine learning models involves adjusting the model parameters based on the feedback of the loss function, allowing the model to learn and refine its predictions over time [9,23].

Using data, models, and loss functions, machine learning systems can learn from experience, adapt to new information, and make informed predictions, distinguishing them from traditional rule-based expert system approaches.

4.2. Machine Learning Categories

Machine learning can be broadly categorised into several types based on the nature of the data and the learning process. The primary types of machine learning include supervised learning, unsupervised learning, reinforcement learning, semi-supervised learning, and self-supervised learning as shown in Figure 4. Since supervised learning involves training models on input–output pairs, surrogate models are developed using this paradigm (i.e., using known data to predict complex system behaviours efficiently). This review will primarily focus on supervised learning, as surrogate models are typically classified within this category.

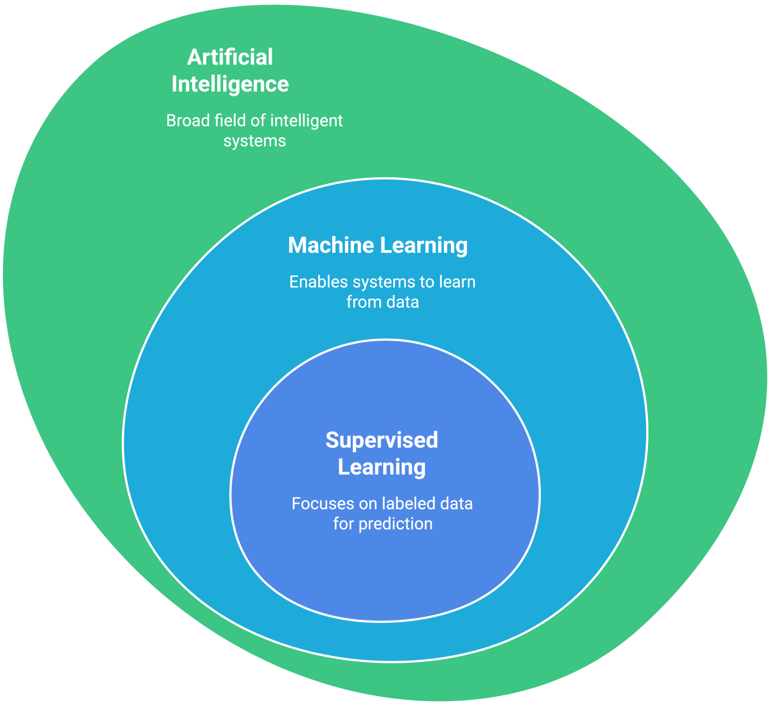

Figure 4. A Venn diagram illustrating the relationship between artificial intelligence, machine learning, and supervised learning.

Supervised learning is a type of machine learning where algorithms learn from labelled data [24]. In this context, labelled data consists of input–output pairs, where the output variable is known. The primary goal of supervised learning is to build a model that can accurately predict the output for new, unseen data based on the patterns learned from the training data.

Common tasks in supervised learning include the following:

- Classification:This involves categorizing input data into predefined classes. In the food industry, surrogate models can be used to classify food quality during packaging processes. For example, in the packaging of processed foods, sensors collect data on parameters like moisture content, temperature, and packaging conditions. A surrogate model, trained using supervised learning, could be developed based on historical process data to predict whether a batch of packaged food meets quality standards based on input variables. In the manufacturing industry, surrogate models can be used for fault classification in assembly line operations to optimise production [25]. For example, a surrogate model can be developed using supervised learning on historical data collected from various sensors installed along the assembly line. The model learns to predict faults based on the data and classifies them into different categories, such as "Minor Misalignment", "Severe Defect", or "No Fault".
- Regression: This task focuses on predicting continuous output variables [22,23]. An example of regression in the manufacturing industry is predicting the surface roughness of a machined part based on features such as cutting speed, feed rate, tool wear, and material hardness. The model aims to map these input parameters related to the machining process to a continuous output variable, which is the surface roughness of the final product.

Supervised learning methods require the value of the output variable for each training sample to be known, allowing for performance evaluation through metrics such as accuracy, precision, and recall [23]. Surrogate modelling is fundamentally a regression problem as it focuses on capturing the relationship between input variables and output responses in complex systems. Surrogate models learn to approximate these relationships by leveraging data from simulations or physical experiments, enabling rapid and efficient predictions for new inputs.

4.3. Machine Learning Techniques for Surrogate Modelling

Machine learning techniques are grounded in statistical principles and computational theories, allowing for the extraction of patterns and insights from large datasets. The process typically involves several key steps, including data collection, data preprocessing, model selection, model training, and model evaluation. During training, algorithms adjust their parameters based on the input data to minimise prediction errors, often utilising techniques such as gradient descent or regularisation to enhance performance. Feature engineering usually plays a crucial role in this process, as it involves selecting and transforming input variables to improve model accuracy. Additionally, the choice of algorithm—ranging from linear regression and decision trees to more complex neural networks—depends on the nature of the data and the specific problem being addressed. As machine learning continues to evolve, the integration of automated machine learning (AutoML) tools can streamline the process of model selection and hyperparameter tuning, making these techniques more accessible to practitioners across various fields [23,26].

The subsequent sections discuss some frequently employed machine learning strategies for developing surrogate models.

4.3.1. Support Vector Regression Models

Support vector regression (SVR) is a supervised machine learning technique used for regression tasks, extending the principles of support vector machines (SVMs), which were originally designed for classification. SVR is particularly effective in handling high-dimensional data and modelling non-linear relationships through the use of kernel functions [27].

SVR formulates an optimisation problem to learn a regression function that maps the input predictor variables to the output observed response values. The primary goal of SVR is to find a function $f(x)$ that has at most an ϵ deviation from the actual target values y_i for the training data, while also being as flat as possible as shown in Figure 5. This is achieved by minimising a loss function that incorporates both the prediction error and the model's complexity [27].

In wine, beer, and yoghurt fermentation processes, SVR can model the non-linear relationship between process variables, such as temperature, pH, and time, and also product quality outcomes, including flavour and alcohol concentration. In a winery, the SVR can predict the ideal duration and temperature of fermentation to achieve the preferred flavour profile and the concentration of alcohol in the end product, using historical fermentation data [28].

Furthermore, SVR's kernel flexibility enables integration with multi-fidelity modelling frameworks, where low-fidelity simulation data can be fused with sparse high-fidelity experimental measurements to improve prediction accuracy without excessive computational cost [29].

However, the performance of SVR as a surrogate model is highly sensitive to the choice of kernel type, regularisation parameter value, and kernel-specific hyperparameters. Hyperparameter tuning methods such as grid search, Bayesian optimisation, and evolutionary algorithms have been successfully employed to optimise these settings for food process applications [30]. Although SVR can produce excellent accuracy, its scalability to very large datasets is limited compared to deep learning models, making it most suitable for small- to medium-sized datasets typical of laboratory-scale and pilot-plant studies.

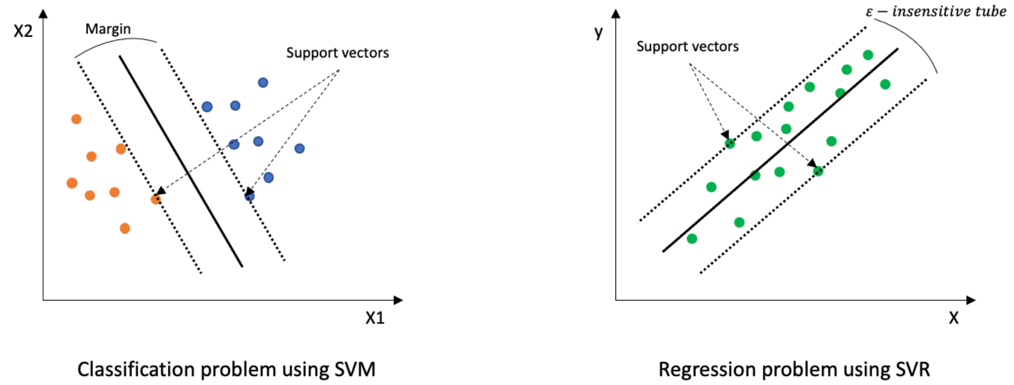

Figure 5. Comparison between a classification problem using support vector machines (SVMs) and a regression problem using support vector regression (SVR). The left diagram illustrates the SVM classification, with a margin separating the support vectors. The right diagram shows the SVR regression with support vectors and the ϵ-insensitive tube.

4.3.2. Gaussian Process Regression

Gaussian processes (GPs) represent a robust non-parametric Bayesian approach used for regression and classification tasks, especially in fields such as machine learning, statistics, engineering, and computational materials science. Gaussian processes provide a flexible framework for modelling complex functions and capturing uncertainty in predictions [31,32].

A Gaussian process (GP) as shown in Figure 6, is a collection of random variables, any finite number with a joint Gaussian distribution [31,32].

Gaussian process regression (GPR) can serve as an effective surrogate modelling tool within the food and drink sector, providing real-time predictions of process variables and capturing system dynamics. The uncertainty estimation from GPR allows for more robust monitoring [33]. GPR has been successfully applied across diverse food processes. For example, it has been used to model drying kinetics of fruits and vegetables, capturing nonlinear moisture–temperature interactions more accurately than polynomial regression [34]. In beer brewing, GPR has been used to predict alcohol yield and sensory attributes based on fermentation conditions, offering uncertainty estimates that inform process adjustments [35]. In dairy processing, GPR has supported the online prediction of cheese ripening indices, such as pH, proteolysis, and texture, from near-infrared spectroscopy data, enabling non-destructive quality monitoring [36].

Beyond these applications, a further advantage of GPR lies in its strong performance in multi-fidelity frameworks, where sparse high-fidelity experimental data are combined with lower-fidelity simulation or pilot-scale data. This has been shown to reduce the need for expensive experimentation in optimisation of spray drying processes and flavour encapsulation [37]. However, scalability remains a limitation, as the complexity of GPR training grows cubically with dataset size. Sparse GPR methods, point approximations, and variational inference approaches are being increasingly explored to extend their applicability to large-scale industrial datasets [38].

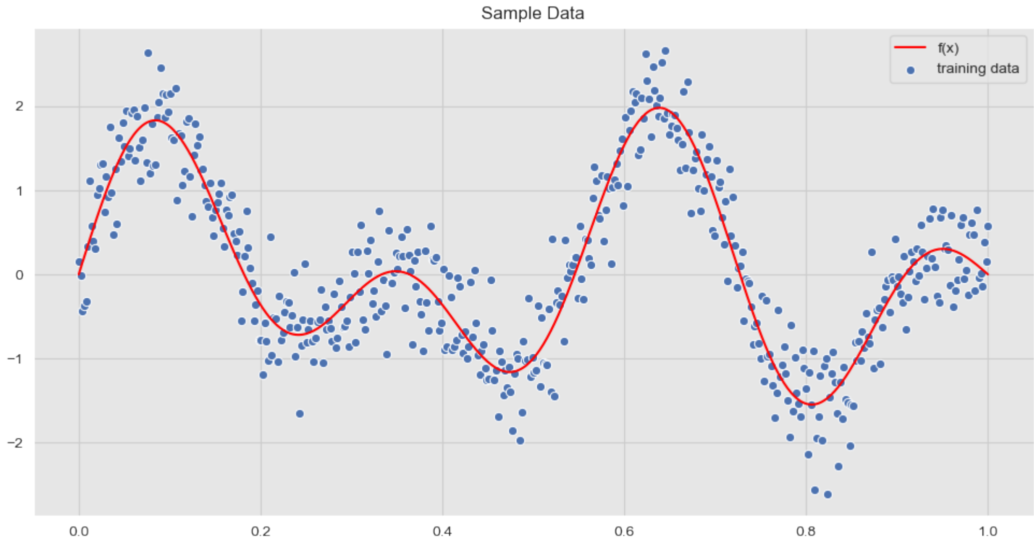

Figure 6. Generated sample data: The red line represents the function $f(x)$ that models the data, while the blue dots represent the training data points.

4.3.3. Artificial Neural Networks

Artificial neural networks (ANNs) are computational models inspired by the biological neural networks that constitute the brains of animals. They are designed to recognise patterns, classify data, and perform various tasks that require learning from examples. ANNs as shown in Figure 7, consist of interconnected groups of artificial neurons that process information using a connectionist approach [39].

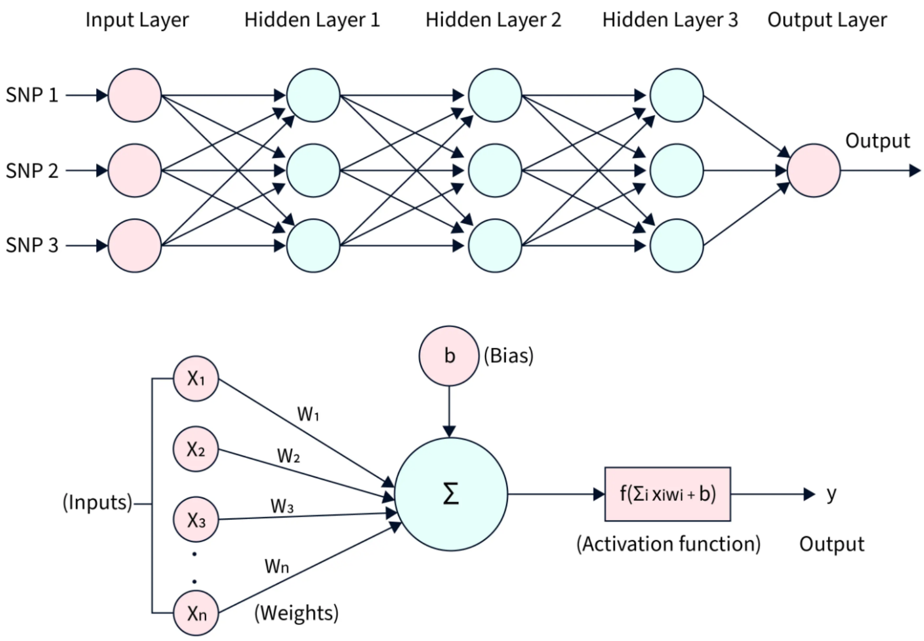

Figure 7. Structure of a feedforward neural network and a single neuron's mechanism. The network consists of an input layer (SNP), multiple hidden layers, and an output layer, where each neuron computes its output using weighted inputs, a bias term, and an activation function.

The basic building block of an ANN is the artificial neuron, which mimics the function of a biological neuron. Each neuron receives inputs, processes them, and produces an output. A weighted sum of the inputs determines the output passed through a non-linear activation function [40].

The learning process in ANNs involves adjusting the weights based on the error between the output and the expected result. One of the most common learning algorithms is the back-propagation algorithm, which uses gradient descent to minimise the error function.

There are various architectures of ANNs, each suited for different types of tasks. The feedforward neural networks are the simplest type of ANNs, where connections between the nodes do not form cycles. Information moves in one direction, from input to output [40].

Feedforward neural networks (FNNs), the most basic form of artificial neural networks (ANNs), have been widely used as surrogate models in food and drink manufacturing. In an FNN, information flows unidirectionally from the input layer through one or more hidden layers to the output layer, without feedback connections. This architecture is well-suited for mapping static, nonlinear input–output relationships that arise in many food processes [41].

ANNs are widely used for predictive maintenance, allowing food and drink manufacturers to forecast equipment failures based on historical sensor data [42]. In a beverage bottling plant, an ANN can predict when machinery will need maintenance by analysing vibration, temperature, and usage data. This ensures that parts are serviced before they break down [43].

In the food and drink sector, ANN-based surrogate models have been successfully applied to predict thermal profiles in pasteurisation, optimise spray drying parameters for powdered products, forecast fermentation yields, and model the rheological properties of beverages. For example, multilayer perceptron (MLP) models have outperformed traditional regression methods in predicting moisture content and texture changes during drying, especially when combined with dimensionality reduction techniques such as principal component analysis (PCA) [44]. Convolutional neural networks (CNNs), a specialised ANN architecture, have been adapted for surrogate modelling in machine vision-based quality control, allowing rapid assessment of product defects from process line images [45].

However, ANN surrogates face challenges in interpretability, risk of overfitting with small datasets, and sensitivity to hyperparameter choices, number of layers, learning rate, and activation functions. Strategies to mitigate these issues include early stopping, dropout regularisation, and integration of physics-based constraints to form physics-informed neural networks (PINNs). In food manufacturing, hybrid ANN–mechanistic models have shown promise by leveraging the generalisation capability of neural networks while retaining the interpretability of domain equations [46].

4.4. Advantages and Limitations of AI-Based Surrogate Modelling

AI-based surrogate models are computational models that utilise artificial intelligence techniques, particularly machine learning algorithms, to approximate complex functions or systems. Unlike traditional surrogate models, which often rely on simpler mathematical forms, such as polynomial regression or Gaussian processes, AI-based models can capture intricate relationships within data through advanced techniques, including neural networks and decision trees [47]. This allows AI-based surrogate models to model non-linearities and interactions more effectively than traditional approaches, making them particularly useful in high-dimensional spaces.

AI-based surrogate models significantly enhance computational efficiency by providing rapid approximations of expensive simulations. Full-scale simulations, such as those used in computational fluid dynamics (CFD) or finite element analysis (FEA), can be computationally intensive and time-consuming. In contrast, once trained, AI-based surrogates can deliver predictions in a fraction of the time, enabling faster iterations in optimisation processes [19]. This efficiency is particularly beneficial in scenarios where multiple evaluations are required, such as in optimisation or uncertainty quantification tasks.

AI-based surrogate models are generally better equipped to handle high-dimensional and complex datasets. Traditional surrogate models often struggle with the "curse of dimensionality", where the volume of the input space increases exponentially with the number of dimensions, making it challenging to sample effectively [48]. AI techniques, particularly deep learning, can learn hierarchical representations of data, allowing them to manage and extract meaningful patterns from high-dimensional spaces more effectively. This capability enables AI-based models to provide accurate approximations even when the underlying relationships are complex and non-linear [19].

AI-based surrogate models exhibit a high degree of adaptability to various domains and changing conditions. Their flexibility enables them to be trained on diverse datasets from various fields, including engineering, aerospace, and manufacturing [12]. Moreover, they can be retrained or fine-tuned with new data to accommodate changes in the underlying processes or conditions, making them suitable for dynamic environments. This adaptability is crucial in applications where system behaviour may evolve over time or under different operational scenarios [19].

AI-based surrogate models can effectively integrate with hybrid methods, including physics-informed models and domain-specific knowledge, to enhance their predictive capabilities. By incorporating physical laws or constraints into the training process, these models can enhance their predictive capabilities while ensuring that the results remain consistent with known scientific principles [47]. This integration enables the development of more robust models that leverage both data-driven insights and established theoretical frameworks, resulting in improved accuracy and reliability in predictions [49].

The performance of AI-based surrogate models heavily depends on the quality and quantity of the training data. High-quality, representative datasets are essential for training models that generalise well to unseen scenarios. However, obtaining sufficient data can be challenging, especially in fields where data collection is expensive or time-consuming [19]. Additionally, issues such as noise, outliers, and missing values can adversely affect model performance. Ensuring that the training data captures the full range of operating conditions is critical for developing reliable surrogates [48].

Interpretability is a significant concern with many AI-based surrogate models, particularly those employing complex architectures, such as deep neural networks. While these models can provide high accuracy, their "black-box" nature makes it challenging to understand how they arrive at specific predictions [49]. This lack of transparency can pose significant challenges in decision-making, particularly in safety-critical applications where understanding the rationale behind a model's output is crucial. The inability to interpret model behaviour may lead to a lack of trust among stakeholders and complicate regulatory compliance [19].

Training AI-based surrogate models, particularly for large-scale problems, can incur substantial costs. These costs arise from several factors, including the need for high-performance computing resources, the time required for model training, and the expertise needed to develop and validate the models [50]. Furthermore, the iterative nature of AI models can lead to increased computational expenses. Organisations must weigh these costs against the potential benefits of improved efficiency and accuracy when considering the adoption of AI-based surrogate modelling.

5. State-of-the-Art Techniques in Surrogate Modelling

This section distinguishes between *neural architectures* (e.g., CNNs, RNNs) and *training paradigms* (e.g., physics-informed training). Section 5.1 will examine and introduce physics-informed neural networks (PINNs) as a training paradigm and provide representative applications in food and drink manufacturing, which incorporate knowledge of the governing equations into the modelling process to enhance the fidelity of the predictions. The remaining subsections will present CNNs and RNNs, explaining what they are and their applications in surrogate modelling.

CNNs and RNNs are neural *architectures* tailored to spatial (grid/image-like) and temporal (sequence) data, respectively. By contrast, a physics-informed neural network (PINN) is not a distinct architecture, but a *training paradigm* that imposes governing physics (e.g., PDEs, conservation laws) via the loss function and can be applied to various architectures (FNN/CNN/RNN/transformers). In the remainder of Section 5, CNNs/RNNs are presented as architectural baselines that may or may not be trained under physics-informed constraints.

5.1. Physics-Informed Neural Networks (PINNs) in Surrogate Modelling

Physics-informed neural networks (PINNs) represent a significant advancement in the field of surrogate modelling, particularly for problems governed by partial differential equations (PDEs). By directly integrating physical laws into the training process of neural networks, PINNs provide a robust framework for approximating complex systems, ensuring that the solutions adhere to the underlying physics [51,52]. PINNs solve supervised learning problems while respecting the underlying physics, making them particularly suitable for modelling systems where labelled data are scarce but physical knowledge is well established [53]. This enables the model to maintain physical consistency during training, offering improved generalisation and interpretability compared to black-box networks.

In food and drink manufacturing, PINNs are gaining traction for their ability to model thermophysical and biochemical processes that are otherwise computationally expensive or analytically intractable.

The architecture illustrated in Figure 8 above comprises four main components of a physics-informed neural network (PINN) framework: (a) Domain variables, such as time and position, serve as inputs. (b) The neural network, represented by a set of hidden layers, parameterised by θ, approximates the target function. (c) Design variables provide additional information, including control parameters like force and power. (d) Loss computation is performed based on the governing equations, constraints, and goals. Automatic differentiation is used to compute derivatives of the output with respect to inputs, ensuring adherence to physical laws. The optimisation seeks to minimise a composite loss function by combining physics laws, constraints, and goals.

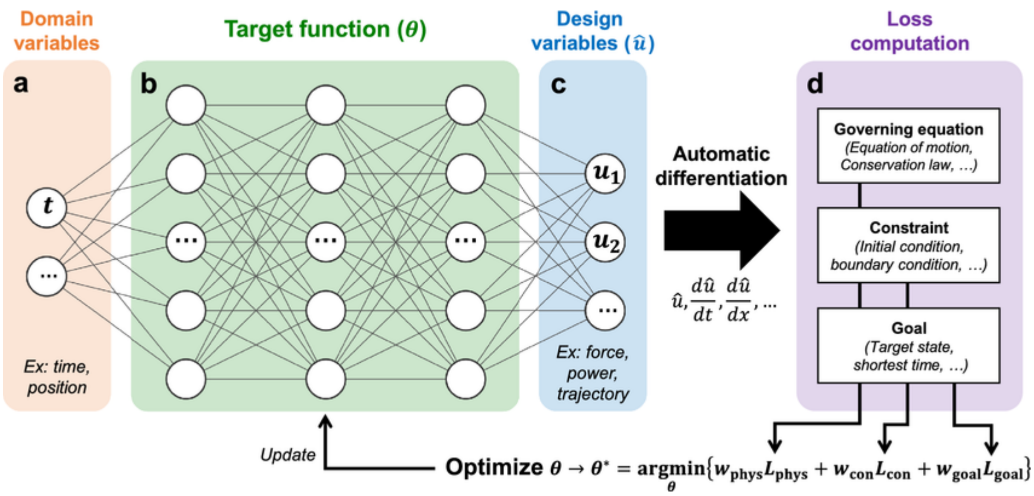

Figure 8. Diagram of a physics-informed neural network (PINN) framework. (Source: Oluwafemidiakho, exploring the capabilities of physics-informed neural networks (PINNs).

PINNs leverage the power of deep learning while incorporating physical knowledge, which allows them to learn from both data and the equations governing the physical behaviour of the system [51]. The fundamental idea of PINNs is to embed the PDEs, along with initial and boundary conditions, into the loss function of the neural network. This approach not only enhances the accuracy of the model but also improves its interpretability and generalisability [54].

The training of a PINN involves minimising the total loss function using optimisation algorithms such as Adam or stochastic gradient descent. The use of automatic differentiation enables the efficient computation of the derivatives required for evaluating the residuals, as highlighted in the literature [55]. The automatic differentiation technique is employed to compute the gradients of the loss function with respect to the network parameters, allowing for efficient backpropagation [56].

During the training process, the network learns to approximate the solution to the PDE while simultaneously fitting the observed data. This dual learning mechanism ensures that the model remains physically consistent, even in the presence of noisy or sparse data.

PINNs have been successfully applied in various fields for surrogate modelling, particularly in scenarios where traditional numerical methods are computationally expensive. For example, in the context of fluid dynamics, PINNs have been utilised to model complex flow phenomena governed by the Navier-Stokes equations [57]. The ability to incorporate physical constraints directly into the model allows for accurate predictions with significantly reduced computational costs.

Physics-informed neural networks (PINNs) have been applied to model transient heat transfer phenomena in pasteurisation and sterilisation processes, where precise thermal profiling is essential for ensuring microbial inactivation without compromising nutritional or sensory quality. In these thermal operations, achieving a uniform temperature distribution throughout the food matrix is vital to avoid both under-processing, which poses food safety risks, and over-processing, which leads to energy inefficiency and product degradation, by embedding the heat conduction equation as a constraint within the PINN framework. Research by Singh et al. was able to generate high-resolution spatiotemporal temperature predictions using sparse sensor data. This enables real-time thermal mapping of food products within retorts and continuous flow systems, facilitating adaptive process control and optimisation. Moreover, PINNs have demonstrated robustness in handling variable boundary conditions, such as fluctuating inlet temperatures and changes in product geometry, making them a versatile surrogate modelling tool for thermal food process engineering [58].

Khan et al. applied physics-informed neural networks (PINNs) to model coupled heat and mass transfer during the drying of biological materials, providing a novel approach for simulating internal moisture content and temperature profiles in food matrices. Drying processes involve complex transient dynamics, particularly when dealing with porous and heterogeneous food products, making conventional numerical techniques such as finite-element methods computationally demanding. In contrast, the PINN framework in this study directly incorporated the governing partial differential equations for moisture diffusion and thermal conduction into the neural network's loss function. This enabled accurate, mesh-free predictions of spatial and temporal moisture and temperature fields using limited experimental data. The model demonstrated lower error margins and faster computation times compared to classical solvers, while maintaining physical consistency. Such capabilities are essential for optimising drying parameters in industrial food manufacturing, where product variability, ambient fluctuations, and energy efficiency are critical considerations. Additionally, the PINN approach showed flexibility in adapting to different geometries, drying conditions, and food substrates, illustrating its potential as a generalisable surrogate modelling tool in the food processing industry [59].

Precision fermentation illustrates how AI-driven surrogate models and advanced control deliver tangible benefits. Predictive control of the model, combined with dynamic flux balance analysis, has improved fed-batch performance in both microbial and mammalian systems. Surrogate models accelerate design space exploration and can be embedded into flowsheet optimisation. Furthermore, machine learning-assisted computational fluid dynamics (CFD) promises faster and more scalable mixing and aeration studies for scale-up. Integrating techno-economic analysis and life cycle assessment in optimisation aligns process choices with cost and sustainability targets [60].

In the context of Bayesian inverse problems, PINNs can serve as surrogate models that facilitate efficient sampling of the posterior. By constructing a surrogate of the forward model using PINNs, researchers can achieve accurate posterior information with a minimal number of forward simulations, as demonstrated in [61].

The integration of physics into the neural network training process offers several advantages, as follows:

- Improved Accuracy: By enforcing physical laws, PINNs can produce more accurate predictions compared to purely data-driven models [54].
- Reduced Data Requirements: PINNs can effectively learn from limited data by leveraging the underlying physics, making them suitable for applications where data collection is expensive or impractical [62].
- Enhanced Interpretability: The explicit incorporation of physical constraints allows for better understanding and interpretation of the model's predictions [55].

Physics-informed neural networks represent a powerful tool for surrogate modelling, particularly in complex systems governed by PDEs. By combining the strengths of deep learning with the rigour of physical laws, PINNs provide a framework that enhances predictive accuracy and ensures that the solutions are physically plausible.

Despite their promise, physics-informed neural networks (PINNs) often require substantial computational resources during training. They are notably sensitive to how different components of the loss function are weighted, particularly the physics-based residual versus data-driven error terms. Recent work has introduced adaptive weighting mechanisms to address this challenge. For example, Wang et al. developed a formulation based on maximum likelihood that dynamically adjusts loss weights during training to enhance convergence and robustness compared to standard PINN [63]. Additionally, Chen et al. proposed a self-adaptive, point-wise weighting method that balances residual decay rates, significantly enhancing prediction accuracy and reducing training uncertainty [64]. Research by Perez et al. into Bayesian PINNs further explores uncertainty quantification in multitask and multiscale settings, automatically tuning loss weights based on task uncertainty to achieve stable and interpretable performance [65].

5.2. Convolutional Neural Networks (CNNs)

Convolutional neural networks (CNNs) are a specialised class of deep learning algorithms designed for processing structured grid data, such as images. They consist of multiple layers, including convolutional layers, pooling layers, and fully connected layers, which work together to extract and learn features from the input data. CNNs are particularly effective in recognising patterns and structures in visual data, making them suitable for various applications in the food and drink sector, such as food image recognition and quality assessment [66].

The architecture of a typical CNN as shown in Figure 9, mimics the connectivity pattern of neurons in the human visual cortex, allowing it to learn hierarchical representations of data. The convolutional layers apply filters to the input data, capturing local patterns, while pooling layers reduce dimensionality, retaining only the most significant features [67]. This ability to learn from large datasets and generalise well to unseen data has made CNNs a popular choice in the food industry for tasks such as food identification and quality detection [68].

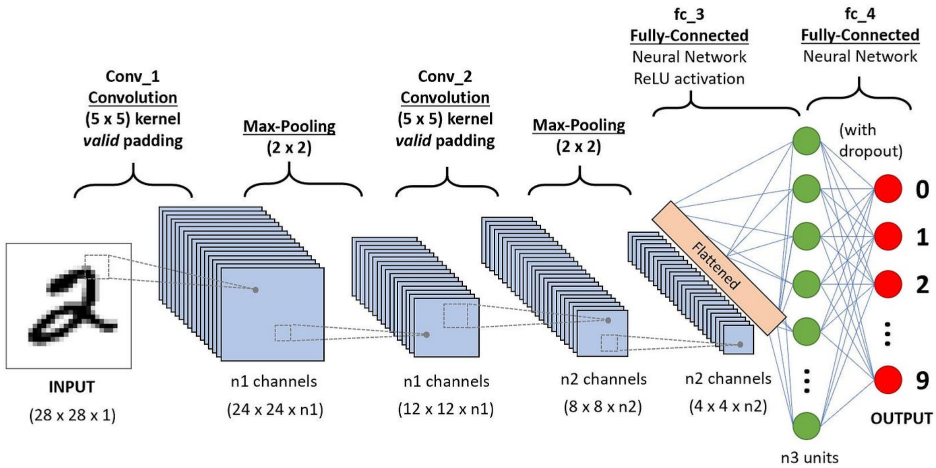

Figure 9. Diagram of a convolutional neural network (CNN) architecture.

CNNs can effectively model complex physical and chemical processes in food production by leveraging their capacity to learn intricate patterns from high-dimensional data. For example, CNNs have been employed to analyse spectral data obtained from techniques like near-infrared (NIR) spectroscopy, enabling the prediction of quality attributes in food products [69]. This approach allows for the identification of key chemical components and their interactions during food processing. Moreover, CNNs can analyse images captured at various stages of food production. By training on labelled datasets that include images of food products at different quality levels, CNNs can learn to identify defects, assess ripeness, and predict shelf life [70]. This capability is crucial for ensuring consistent product quality and optimising production processes. Research has demonstrated that CNN-based surrogate models can capture the dynamics of food production processes by integrating data from multiple sources, including chemical composition and environmental conditions [71].

For example, in a bottling line, CNNs can analyse images of bottle caps to classify them as usual, unfixed, or missing, ensuring quality control and reducing waste [72]. Additionally, CNNs can predict the remaining shelf life of products based on real-time data, assisting manufacturers in making informed decisions about inventory management and distribution [70].

Integrating CNN surrogate models with sensors and Internet of Things (IoT) systems facilitates real-time monitoring and optimisation of food production processes. By connecting sensors that measure various parameters such as temperature, humidity, and chemical composition to a CNN model, manufacturers can continuously feed data into the model for analysis [72]. This real-time data integration can allow for immediate feedback on production conditions, enabling on-the-fly adjustments to optimise processes in the food and drink manufacturing industry. The use of IoT systems enhances this integration by providing a platform for data collection, storage, and analysis, allowing food manufacturers to gain insights into their production processes and implement predictive maintenance strategies [71].

To address the limitations of CNNs in food production, several potential advancements can be explored. One approach is the development of hybrid models that combine CNNs with other machine learning techniques, such as recurrent neural networks (RNNs) or reinforcement learning. This combination could enhance the model's ability to capture temporal dynamics and improve predictive accuracy. Additionally, incorporating transfer learning techniques can help mitigate the data scarcity issue by allowing models trained on large datasets from related domains to be fine-tuned for specific food production tasks. This approach can significantly improve CNN performance in food detection and analysis [71].

5.3. Recurrent Neural Networks (RNNs)

Recurrent neural networks (RNNs) are a class of artificial neural networks designed to recognise patterns in data sequences, such as time series or natural language [73]. Unlike traditional feedforward neural networks, RNNs have connections that loop back on themselves, allowing them to maintain a hidden state and capture information about previous inputs [74]. This unique architecture enables RNNs to model temporal dependencies and sequential data effectively.

The basic structure of an RNN consists of input, hidden, and output layers as shown in Figure 10. The hidden layer retains information from previous time steps, which is crucial for tasks where context is essential [75]. For example, in the food industry, RNN can be used to analyse time-dependent data such as temperature, humidity, and other environmental factors that influence food quality and safety [76].

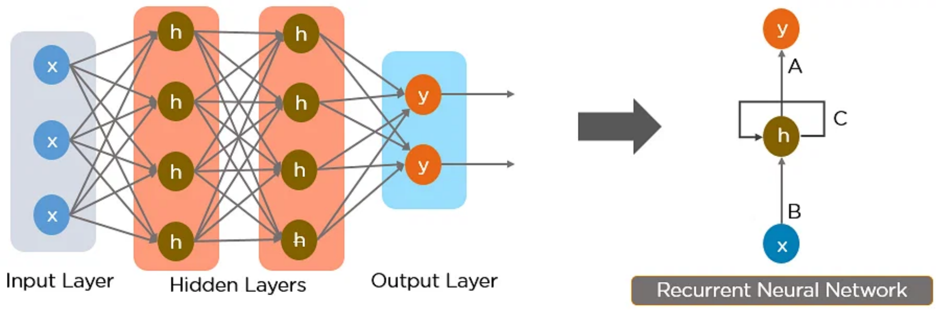

Figure 10. Diagram of a recurrent neural network (RNN) architecture.

Recurrent neural networks (RNNs) are particularly well-suited to model complex physical processes in the food industry because of their ability to handle sequential data and learn from historical patterns [77]. They can be applied in various areas, including the following:

- Quality Control: RNNs can predict the quality of food products based on historical data, such as temperature and humidity during processing. For example, they can model the fermentation process in dairy production, where various time-dependent factors influence the quality of the final product [76].
- Process Optimization: By analysing historical data, RNNs can identify optimal processing conditions. For example, they can be used to optimise drying processes by predicting the moisture content over time, ensuring that products are dried to the desired specifications without compromising quality [46].
- Predictive Maintenance: RNNs can forecast equipment failures by analysing time-series data from sensors monitoring machinery. This predictive capability enables timely maintenance, reducing downtime and enhancing operational efficiency [78].

RNNs can process incoming data streams to provide immediate feedback on production processes. For example, in a brewing process, RNNs can analyse fermentation data in real time to dynamically adjust conditions, ensuring optimal flavour and quality [79]. By integrating RNNs with IoT systems, food manufacturers can develop decision support systems that provide actionable insights based on real-time data analysis. These systems can help make informed decisions about process adjustments, resource allocation, and quality control.

Using advanced RNN architectures such as long-short-term memory (LSTM) networks and gated recurrent units (GRUs) can help mitigate the vanishing gradient problem and improve the model's ability to capture long-term dependencies [80].

Recurrent neural networks, particularly LSTM and GRU architectures, have significant potential as surrogate models in the food and drink sector. Their ability to model complex physical processes, integrate with IoT systems for real-time monitoring, and optimise production processes can lead to enhanced efficiency and sustainability in food production. In food processing environments, where real-time data is continuously generated from sensors, such as temperature, pH, moisture content, and machine vibration, RNN-based models can act as efficient surrogates for complex, physics-based simulations. These models can learn intricate patterns and relationships from data, enabling accurate predictions of process outcomes, product quality, and equipment behaviour. As research and technology continue to advance, the application of RNNs in the food and drink sector is likely to expand, paving the way for more innovative and sustainable food production practices.

6. Application of Surrogate Models in the Food and Drink Manufacturing Industry

This section provides an overview of the food and drink manufacturing industry, including its challenges, and how surrogate models can be utilised to address these issues. The first subsection will discuss the variability in raw materials and its impact on product quality and process efficiency, illustrating how surrogate models can improve decision-making and process control. Next, we will examine the computational challenges of simulating complex food processes and explore how surrogate models can provide efficient solutions.

6.1. Food and Drink Manufacturing Challenges

The food and drink manufacturing industry faces several key challenges that can be effectively addressed through the application of surrogate models. One significant challenge is the inherent variability in raw materials, which can lead to inconsistencies in product quality and process efficiency. Surrogate models can help predict results based on limited experimental data, facilitating better decision-making and process control [81]. For instance, in processes such as fermentation and baking, where the interactions between ingredients and environmental conditions are complex, surrogate models can optimise conditions to enhance product quality while minimising resource use [82].

Another major challenge in the food and drink sector is the computational intensity of simulating complex food processes. Traditional modelling approaches often require extensive computational resources, making them impractical for real-time applications. Surrogate models, which are simpler approximations of complex systems, can significantly reduce computational demands while maintaining accuracy in scenarios requiring numerous simulations, such as optimisation studies or Monte Carlo simulations [82]. Specific processes in food and drink manufacturing are particularly resource-intensive or complex and can benefit from optimisation using surrogate models. Clean-in-place (CIP) systems, for example, are essential for maintaining hygiene in food processing but often lead to excessive use of water, energy, and cleaning agents [81]. By employing surrogate models, manufacturers can optimise CIP parameters, reducing resource consumption while ensuring effective cleaning *(experiment-calibrated surrogate trained on plant and sensor data)* [81].

Complex interactions among various parameters, including temperature, humidity, and ingredient composition, characterise processes such as baking, fermentation, and drying. Surrogate models can be used to explore these interactions and identify optimal operating conditions, thereby enhancing efficiency and product quality [83].

The primary objectives of the food and drink manufacturing industry include cost reduction, quality improvement, sustainability, and efficiency. Surrogate models can be tailored to address these objectives by enabling manufacturers to explore various operational scenarios and identify optimal conditions for production [83]. For example, surrogate models can help minimise energy usage during baking while ensuring product quality, thus contributing to sustainability goals [81].

Various surrogate models are applicable in food and drink manufacturing, including Gaussian processes, neural networks, and polynomial chaos expansions. These models are beneficial for capturing the complex relationships between input parameters and output in food processes. For example, neural networks can be used to model the relationship between ingredient properties and final product quality, allowing predictive analytics in product development. Training surrogate models typically requires data sets that cover a range of operating conditions and product characteristics, often derived from historical data or designed experiments [81]. The quality and quantity of data used for training are critical as they directly impact the performance of the surrogate model.

Physical and chemical processes in food manufacturing, such as mixing, baking, and fermentation, require physics-informed surrogate models. These models integrate fundamental physical principles with empirical data to improve predictive accuracy. For example, in baking, surrogate models can be used to predict the effects of temperature and humidity on the texture and taste of the product, thus optimising the baking process [82]. In the food and drink manufacturing sector, the optimisation of clean-in-place processes and the application of Bayesian optimisation techniques have been used to minimise water and energy consumption while maintaining hygiene standards. In addition, surrogate models have been utilised in quality control applications, such as predicting taste, texture, and shelf life based on ingredient variability [81].

Surrogate models play a crucial role in mitigating variability in raw materials or production conditions. By modelling the relationships between processing conditions and product stability, manufacturers can make informed decisions that enhance food safety and extend shelf life [83]. This capability is particularly valuable in industries where the quality of raw materials can fluctuate significantly, such as in the production of beverages and baked goods [81].

The integration of surrogate models with Industry 4.0 technologies represents a significant advancement in the food and drink manufacturing sector. Industry 4.0 encompasses a range of technologies, including the Internet of Things (IoT), artificial intelligence (AI), big data analytics, and digital twins, all of which can enhance operational efficiency, product quality, and sustainability in food production processes. By integrating data from various sources, including historical production data and real-time monitoring, surrogate models can provide insights into how changes in processing conditions affect product stability and safety [83].

Digital twins are virtual replicas of physical systems that allow for real-time monitoring and simulation of processes. Surrogate models play a crucial role in developing digital twins by providing simplified representations of complex systems, enabling faster computations and real-time decision-making. By integrating surrogate models into digital twins, manufacturers can simulate various scenarios, optimise processes, and predict outcomes without the need for extensive physical trials. This capability is particularly valuable in the food industry, where the complexity of processes and variability in raw materials can make traditional modelling approaches cumbersome and time-consuming [14].

The IoT facilitates the collection of vast amounts of data from sensors embedded in production equipment and processes. Surrogate models can be used to analyse this data, providing insights into process performance and enabling predictive maintenance. For instance, in aquaculture, IoT devices can monitor water quality parameters, and surrogate models can predict fish growth based on these parameters, allowing for optimised feeding schedules and resource management [84]. This integration not only improves operational efficiency but also reduces waste and enhances sustainability by ensuring that resources are used effectively.

The integration of surrogate models with Industry 4.0 technologies allows for the utilisation of real-time data in decision-making processes. By continuously updating surrogate models with data collected from IoT devices, manufacturers can adapt their operations to changing conditions, ensuring optimal performance [81].

Surrogate models can be enhanced by applying AI and machine learning techniques. These technologies can be employed to refine surrogate models by identifying patterns in data that may not be immediately apparent [85].

Despite the potential benefits of integrating surrogate models with Industry 4.0 technologies in the food and drink sector, several challenges remain. The complexity of food processes and the variability of raw materials can complicate the development and implementation of effective surrogate models [86]. Additionally, the need for high-quality data to train these models is critical, as inaccuracies in the data can lead to suboptimal predictions and decisions [87]. Future research can focus on developing robust data collection and management strategies, as well as exploring the application of advanced machine learning techniques to enhance the capabilities of surrogate models within the context of Industry 4.0.

6.2. Process Optimisation in the Food Sector Using Surrogate Modelling

The food sector faces numerous challenges in process optimisation, primarily revolving around efficiency, quality control, and cost reduction. Achieving optimal efficiency in production processes is critical, as it directly impacts throughput and operational costs. The complexity of food processes, which often involve multiple variables and interactions, complicates the identification of the most efficient operational parameters [88]. Quality control is paramount, as variability in raw materials and processing conditions can lead to significant quality issues. The need to maintain consistent product quality necessitates robust optimisation strategies [89]. Additionally, the food industry is under constant pressure to reduce production costs while adhering to safety and quality standards, which includes minimising waste and energy consumption [87].

Traditional optimisation methods in the food sector often rely on direct experimentation and empirical models, which can be time-consuming and resource-intensive. Techniques such as gradient-based optimisation are effective for smooth, continuous functions but struggle with complex, non-linear food processes [81]. Heuristic methods, while helpful in exploring large solution spaces, may not guarantee optimal solutions. In contrast, surrogate modelling offers a more efficient approach by creating simplified models that approximate the behaviour of complex systems. Surrogate models can quickly evaluate multiple scenarios without the need for extensive physical experimentation, making them particularly advantageous in the food industry [87].

The primary goals of process optimisation in food manufacturing include yield improvement, waste reduction, and energy efficiency. Maximising the output of desired products from raw materials is crucial, as higher yields correlate directly with profitability. Waste reduction is essential for sustainability and cost-effectiveness, and data-driven models can help identify opportunities for minimising waste in various food processing operations [87]. Furthermore, reducing energy consumption during processing lowers costs and contributes to environmental sustainability, a growing concern in the food sector [88].

The food sector is increasingly adopting advanced optimisation techniques, including data-driven approaches and machine learning. Industry trends indicate a shift towards the integration of IoT and big data for real-time process monitoring and optimisation [90]. Sustainability initiatives are also gaining traction, with a focus on reducing environmental impact through optimised resource use [87]. Automation and robotics are being implemented to enhance precision and efficiency in production, further driving the need for sophisticated optimisation strategies [91].

Several case studies have illustrated the successful application of surrogate models in food production optimisation. For instance, surrogate models have been utilised to optimise the concentration of fruit juices, balancing energy use and product quality [88]. In cleaning-in-place (CIP) processes, Bayesian optimisation combined with surrogate modelling has improved efficiency by minimising water use and energy consumption [81]. Surrogate models can optimise parameters in food formulation by identifying optimal ingredient ratios and reducing the experimental burden. By simulating various formulations, surrogate models minimise the need for extensive physical trials, allowing for quicker product development iteration [91].

6.3. Energy Consumption in the Food and Drink Industry

The food and drink industry is a significant energy consumer, accounting for a substantial portion of total energy consumption in the manufacturing sector. This section examines the primary processes that require energy, the types of energy utilised, the variations between different segments, and the environmental and economic implications of energy consumption in this sector.

Energy consumption in the food and drink industry encompasses various energy-intensive processes. Key processes include electricity, thermal energy, mechanical energy, refrigeration, and cleaning and sanitation. Thermal processing, which includes cooking, baking, and drying, is prevalent in sectors such as food processing and dairy production. For instance, the production of instant coffee and milk powder involves significant thermal energy consumption, with processes like freeze-drying and drying being particularly energy-intensive [92]. Refrigeration is another critical aspect, especially in the beverage industry, where it is recognised as one of the most energy-intensive processes [93]. Additionally, cleaning and sanitation in meat and dairy processing have increased energy and water use due to stringent hygienic standards [92]. Electricity is extensively used in rice milling, refrigeration, lighting, and various processing equipment. Thermal energy, sourced from natural gas, steam, and other fuels, is crucial for cooking and heating processes. Mechanical energy is employed in operations such as mixing, milling, grinding, and packaging. The reliance on fossil fuels remains a concern, as the industry continues to depend on natural gas and petroleum, which are considered unsustainable [92].

Energy consumption varies significantly between different segments of the food and drink industry. For example, the energy consumption for bakery products averages around 5.21 MJ/kg [94]. The brewing industry, particularly beer production, is dominated by small and medium-sized enterprises (SMEs), which account for a significant portion of energy use in this sector [95]. Dairy processing is highly energy-intensive, with an average total specific consumption of 13.8 MJ/kg for cheese and 10.3 MJ/kg for powdered milk [94]. The energy intensity of the meat industry is also notable, with a mean consumption of primary energy of approximately 4.4 MJ/kg for poultry and 3.0 MJ/kg for pig meat [95].

The environmental impacts of energy consumption in the food and drink industry are profound, contributing to greenhouse gas emissions and resource depletion. The sector is responsible for a significant share of the total GHG emissions, necessitating urgent action to improve energy efficiency [96]. Economically, high energy costs can affect profitability, particularly for SMEs that may lack the resources to invest in energy-efficient technologies [97]. The food industry is also facing increasing pressure to adopt sustainable practices, as consumer awareness and demand for environmentally friendly products grow [96]. Cost savings are a significant driver in improving energy efficiency in the food and drink industry, as reducing energy consumption directly correlates with lower operational costs [95]. Additionally, sustainability goals are increasingly influencing companies to enhance their energy efficiency, as consumers demand more environmentally responsible practices [97].

While a growing body of research exists on energy consumption in the food and drink industry, significant gaps remain in the application of surrogate modelling techniques. Specifically, the literature lacks comprehensive studies that integrate surrogate modelling with energy consumption data to predict and optimise energy use in various food processing sectors. The potential of surrogate modelling to bridge the gap between complex energy systems and practical applications in the food industry remains under-explored.

7. Current Challenges and Limitations of Surrogate Modelling

Surrogate modelling has emerged as a powerful tool in various fields, particularly in engineering and optimisation. Despite its advantages, surrogate modelling is not without its challenges and limitations. Below are the common challenges and trade-offs between accuracy and computational efficiency faced in surrogate modelling.

One of the primary challenges in surrogate modelling is ensuring model accuracy, particularly when the surrogate model is built on a limited dataset. Surrogate models are often constructed based on a limited dataset, which can lead to overfitting or underfitting. Overfitting occurs when the surrogate model captures noise in the training data rather than the underlying relationship, resulting in poor generalisation to new data points. Conversely, underfitting happens when the model is too simplistic to capture the complexities of the original model. These issues are often linked to the way the training data is sampled. Inadequate or poorly distributed samples can fail to cover critical regions of the input space, especially in high-dimensional, non-linear systems. To address this, sampling strategies such as Latin hypercube sampling, adaptive sampling, or active learning are crucial for generating informative data points in the design space, which enhances the model's ability to make accurate predictions or inferences on new, unseen data based on the patterns it learned during training. For instance, in the context of chemical process optimisation, surrogate models must accurately represent the non-linear relationships between input parameters and outputs, which can be particularly challenging when dealing with high-dimensional spaces [98].

Another significant challenge is managing uncertainty. Many real-world processes are subject to variability and noise, which can affect the performance of surrogate models. For example, in the optimisation of distillation processes, the presence of numerical noise in the simulation can complicate the development of reliable surrogate models [99]. Researchers have noted that the performance of surrogate models can vary significantly based on the quality and quantity of the training data, as well as the sampling strategies employed [100]. This variability can lead to different realisations of the surrogate model, making it difficult to achieve consistent and reliable predictions.

In wastewater treatment optimisation, surrogate models are used to predict the performance of various treatment configurations. The primary challenge in using surrogate models for wastewater treatment optimisation is ensuring the accuracy of the surrogate in representing the underlying complex processes. The surrogate model must capture the non-linear relationships between input parameters (such as flow rates, concentrations, and operational conditions) and output responses (like effluent quality and treatment efficiency). If the surrogate model is not sufficiently accurate, it may lead to suboptimal decisions in the treatment process [98]. Wastewater treatment processes are inherently subject to variability and uncertainty, including fluctuations in influent characteristics as well as operational conditions. Managing this uncertainty is crucial, as it can significantly impact the performance of surrogate models. For instance, if the surrogate model does not account for the variability in wastewater composition, the optimisation results may not be robust, leading to potential failures in meeting regulatory standards [100]. The performance of surrogate models heavily relies on the quality and quantity of the training data used to build them. In wastewater treatment, obtaining high-fidelity data from simulations or experiments can be resource-intensive and time-consuming. Limited or poor-quality data can result in inaccurate surrogate models, which may not generalise well to unseen scenarios [17]. The choice of sampling methods for generating training data is critical. Traditional methods, such as random sampling or Latin hypercube sampling, may not adequately capture the design space, particularly in high-dimensional problems typical of wastewater treatment optimisation. Advanced design of experiments methodologies are needed to ensure that the surrogate model is trained effectively [101]. While surrogate models are designed to reduce computational costs, the initial development phase can still be expensive, especially when high-fidelity simulations are required to generate training data. The computational burden can be exacerbated when dealing with multi-fidelity models, where the decision on how to allocate computational resources between low- and high-fidelity simulations remains a challenge [101].

Integrating surrogate models with optimisation algorithms can be complex, primarily due to challenges related to model accuracy, variability, and calibration. The optimisation process often requires iterative evaluations of the surrogate model. If the model is not well-calibrated or exhibits high variability, it can lead to convergence issues or inefficient searches for optimal solutions [102]. A critical consideration in surrogate modelling is the trade-off between accuracy and computational efficiency. While surrogate models are designed to provide faster evaluations than high-fidelity simulations, balancing speed and accuracy can be difficult. In many cases, increasing the complexity of the surrogate model—such as using higher-order polynomials or more sophisticated machine learning techniques—can improve accuracy but at the cost of increased computational demands during the training phase. This trade-off is often observed when using complex models, such as Gaussian processes, which yield highly accurate predictions but require more computational resources for training compared to simpler models, like polynomial regression [98]. Moreover, the performance of surrogate models can significantly depend on the quality and quantity of the training data and the sampling strategies employed, which affects their ability to generalise and make reliable predictions [100].

In the aerospace industry, surrogate models are frequently used for aerodynamic shape optimisation. However, the complexity of the flow dynamics and the presence of noise in the simulation data can hinder the accuracy of the model, making it challenging to obtain consistent and reliable results [101]. Similarly, in the optimisation of distillation processes, surrogate models are employed to replace computationally expensive simulations. Yet, numerical noise in the simulations complicates the development of reliable surrogate models, which can lead to inaccuracies and inefficiencies in the optimisation process [99].

In the context of catalytic reforming processes, researchers have found that while complex surrogate models, such as Gaussian processes, can offer highly accurate predictions, they require significantly more computational resources for training compared to simpler approaches, such as polynomial regression [98]. This can be particularly problematic in situations requiring rapid decision-making, such as real-time process control. Similarly, in machine learning applications, specific techniques like support vector machines may not match the accuracy of models like Gaussian Processes but offer faster training times, necessitating a careful selection of the surrogate model based on the specific application and constraints [9].

Reduced order models (ROMs) are also an essential class of surrogate modelling. ROMs simplify complex mechanistic models while retaining their spatio-temporal fidelity, thereby providing fast yet physically grounded predictions. Recent work by Ghosh and Datta (2023) demonstrated a deep-learning–enabled ROM for food processes, where transient heat transfer and coupled heat moisture transport were predicted in real time with high accuracy compared to full finite-element simulations [13]. For example, the ROM successfully modelled thermal sterilisation operations, reproducing temperature profiles at a fraction of the computational cost of high-fidelity PDE solvers. In addition, ROMs were applied to simulate spatio-temporal moisture diffusion during food drying, a process where conventional mechanistic models require significant computational resources due to moving boundaries and strong non-linearities. The deep-learning-enabled ROM approximated the same dynamics while being 100–1000$\times$ faster, enabling near real-time prediction of moisture content evolution. These results highlight the potential of ROMs to serve as reliable digital twin components for online process control and optimisation in food manufacturing.

Despite their advantages, AI-based surrogate models are constrained by several practical limitations. Interpretability remains a major concern, especially for complex neural networks. In food safety applications, black-box predictions hinder trust and regulatory compliance. Reviews call for governance frameworks that address bias, transparency, and equitable access in food and manufacturing deployments [103].

Another challenge lies in hyperparameter optimisation. The performance of models like CNNs and PINNs is susceptible to architecture choices, number of layers, kernel sizes, and regularisation. Grid search, random search, Bayesian optimisation, and AutoML frameworks are increasingly used to tune these settings efficiently.

AI-based surrogate models are often trained on datasets derived from specific production lines or process configurations. Consequently, their ability to generalise to new settings, such as different plant layouts, ingredient compositions, or environmental conditions, is limited. This challenge is being addressed through transfer learning and domain adaptation techniques. However, empirical validation of these strategies in industrial food manufacturing remains sparse, representing an open area of research.

The summary in Table 1 provides a conceptual map of the major surrogate modelling strategies, applications, benefits, and limitations used in food and drink manufacturing. The table offers a structural guide for researchers and practitioners to identify the most suitable approach for specific unit operations or decision-making contexts. For example, data-driven models remain attractive for rapid input–output prediction and monitoring tasks. At the same time, physics-informed approaches, such as PINNs and ROMs, are particularly valuable for maintaining spatio-temporal process fidelity in thermal and drying operations. Hybrid mechanistic–ML models stand out for system-level optimisation and digital twin development, especially when life-cycle assessment or techno-economic objectives are considered.

Table 1. Summary of surrogate modelling approaches in food and drink manufacturing, with methodology context and representative citations.

Approach	Applications in Food & Drink	Benefits	Limitations/Challenges	High-Fidelity Source & ML Framework/Training	Representative Applications
Data-driven models (e.g., RF, GP, ANN)	Fermentation kinetics prediction; quality control (e.g., texture, flavour); wastewater treatment optimisation; CIP optimisation	Easy to train on available data; good accuracy for input–output mapping; useful in monitoring and soft sensors	Risk of over/underfitting with limited data; sensitive to sampling strategy; limited transfer across plants; interpretability concerns	Source: Experimental/plant data (DoE, historical); Framework: RF/GP/ANN; Training: cross-validation, Bayesian/rand search for hyperparameters	CIP optimisation with Bayesian methods [81], wastewater/process optimisation [87,98–100,104], quality prediction [38,66,68–71], energy assessment in juice concentration [88]
Physics-Informed Neural Networks (PINNs)	Thermal processes (pasteurisation, sterilisation); drying (heat–mass transfer); inverse problems; fermentation with pH/temperature coupling	Embed PDEs/constraints into loss; high spatio-temporal fidelity; robust with sparse/noisy data; improved interpretability	Computationally expensive to train; sensitive to loss weighting and hyperparameters; industrial practice still emerging	Source: Mechanistic PDEs + sparse data; Framework: FNN/CNN/RNN/transformers with physics-informed loss; Training: Adam/SGD with adaptive loss weighting, UQ (Bayesian PINNs)	Food thermal/drying modelling [58,59], PINN methodology and advances [51–55,63–65] inverse problems [61]
Reduced Order Models (ROMs)	Drying dynamics (moisture diffusion); CFD-based aeration/mixing; heat transfer in food matrices; sterilisation trajectories	Retain physics fidelity at much lower cost; often 100–1000× faster than full PDE solvers; suitable for near real-time DT	Require careful training/validation; accuracy–efficiency trade-off; reduced flexibility under extreme extrapolation; sampling critical	Source: High-fidelity FEM/CFD simulations; Framework: deep-learning–enabled ROM (autoencoders/operators); Training: supervised on HF snapshots with physics-consistency checks	Deep-learning–enabled ROMs in food processes [13], thermal sterilisation & coupled heat–moisture transport [13], general CAE context [82]
Hybrid Mechanistic–ML Models	Precision fermentation (MPC with dFBA); flowsheet optimisation; process intensification; soft sensors aligned with LCA/TEA	Combine mechanistic interpretability with ML flexibility; system-level optimisation; alignment with sustainability and cost goals	Integration complexity; need diverse datasets; hyperparameter optimisation critical; risk of drift in real-time deployment	Source: Mechanistic cores + data-driven submodels; Framework: hybrid ML (GP/NN) with mechanistic constraints; Training: joint calibration, Bayesian optimisation/AutoML	Precision fermentation & DT integration [60], broader food engineering optimisation [82], AI-in-food reviews [3–5]

8. Conclusions and Further Research Directions

Despite advancements in surrogate modelling techniques, specific gaps remain in the current literature regarding the application of surrogate modelling in the food and drink industry. Most studies are based on specific processes or technologies, thus calling for systematic reviews that encompass surrogate modelling within multiple food manufacturing processes. Also, the capability of surrogate models to support real-time energy management and decision-making has not been further explored.

Future research should focus on the development of more sophisticated surrogate models that can capture the various conditions characterising food production processes. In the food and drink industry, transformers can be utilised in the creation of surrogate models, which are used to make predictions based on various input factors, such as ingredients, cooking techniques, and consumer tastes. Transformers are a class of deep learning models that have significantly advanced the field of natural language processing (NLP) and are increasingly being applied in various domains, including the food and drink industry. Introduced by Vaswani in [104], the Transformer architecture is characterised by its self-attention mechanism, which allows the model to weigh the importance of different input elements dynamically. This capability enables transformers to capture long-range dependencies in data, making them particularly effective for tasks that require understanding context and relationships within sequences. The ability of transformers to process and analyse large datasets makes them suitable for tasks such as predicting nutritional content, assessing food quality, and optimising recipes [105]. Additionally, combining transformers with other machine learning techniques, such as reinforcement learning, could lead to the development of more sophisticated models that not only predict outcomes but also recommend optimal operational strategies based on historical performance data [106].

The integration of machine learning models with surrogate modelling can improve the accuracy of the surrogate models and help estimate energy consumption trends better. Additionally, there is a need for benchmarking methods to determine how surrogate models contribute to enhancing energy efficiency across various segments of the food and beverage industry.

Surrogate modelling, therefore, has the potential of being a valuable tool in enhancing energy efficiency in the food and drink industry. Through the application of advanced modelling approaches, such as sampling and uncertainty quantification, stakeholders will be able to understand the patterns of energy use and, therefore, be in a position to make recommendations that may lead to improved efficiency in the food production chain.

Author Contributions: Conceptualisation, E.L. and A.S.; Methodology, E.L.; Writing—Original Draft, E.L. and A.S.; Writing—Review & Editing, E.L., A.S., and C.E.d.S.; Resources, E.L. and A.S.; Supervision, A.S. and C.E.d.S. All authors have read and agreed to the published version of the manuscript.

Funding: This study received no external funding.

Data Availability Statement: No new data were created or analysed in this study.

Acknowledgments: The authors gratefully acknowledge support from the Advanced Food Innovation Centre (AFIC), the Commonwealth Scholarship Commission (CSC), and Sheffield Hallam University.

Conflicts of Interest: The authors declare that they have no conflicts of interest.

References

1. Raj, M.; Seamans, R. Artificial intelligence, labor, productivity, and the need for firm-level data. In *The Economics of Artificial Intelligence: An Agenda*; University of Chicago Press: Chicago, IL, USA , 2018; pp. 553–565.
2. Ronaghi, M. The Influence of Artificial Intelligence Adoption on Circular Economy Practices in Manufacturing Industries. *Environ. Dev. Sustain.* **2023**, *25*, 14355–14380. [CrossRef]
3. Agrawal, K.; Goktas, P.; Kumar, N.; Leung, M.F. Artificial intelligence in personalized nutrition and food manufacturing: A comprehensive review of methods, applications, and future directions. *Front. Nutr.* **2025**, *12*, 1636980. [CrossRef]
4. Ding, H.; Tian, J.; Yu, W.; Wilson, D.I.; Young, B.R.; Cui, X.; Xin, X.; Wang, Z.; Li, W. The application of artificial intelligence and big data in the food industry. *Foods* **2023**, *12*, 4511. [CrossRef]
5. Mavani, N.R.; Ali, J.M.; Othman, S.; Hussain, M.; Hashim, H.; Rahman, N.A. Application of artificial intelligence in food industry—A guideline. *Food Eng. Rev.* **2022**, *14*, 134–175. [CrossRef] [PubMed]
6. Canatan, M.; Alkhulaifi, N.; Watson, N.; Boz, Z. Artificial Intelligence in Food Manufacturing: A Review of Current Work and Future Opportunities. *Food Eng. Rev.* **2025**, *17*, 189–219 . [CrossRef]
7. Graetz, G.; Michaels, G. *Robots at Work: The Impact on Productivity and Jobs*; Technical Report; Centre for Economic Performance, LSE: London, UK, 2015.
8. Badini, S.; Regondi, S.; Pugliese, R. Unleashing the Power of Artificial Intelligence in Materials Design. *Materials* **2023**, *16*, 5927. [CrossRef] [PubMed]
9. Espinoza Guzmán, J. Study on the Performance of Machine Learning Algorithms as Surrogate Models for a Representative Model. Master's Thesis, Norwegian University of Science and Technology (NTNU), Trondheim, Norway, 2023.
10. Iuliano, E.; Pérez, E. *Application of Surrogate-Based Global Optimization to Aerodynamic Design*; Springer: Cham, Switzerland, 2016; Volume 22.
11. Anlesinya, A.; Dadzie, S.A. Technology and the conduct of bibliometric literature reviews in management: The software tools, benefits, and challenges. In *Advancing Methodologies of Conducting Literature Review in Management Domain*; Emerald Publishing Limited: Leeds, UK, 2023; pp. 57–78.
12. Franzoi, R.; Kelly, J.; Menezes, B.; Swartz, C. An Adaptive Sampling Surrogate Model Building Framework for the Optimization of Reaction Systems. *Comput. Chem. Eng.* **2021**, *152*, 107371. [CrossRef]
13. Ghosh, D.; Datta, A. Deep learning enabled surrogate model of complex food processes for rapid prediction. *Chem. Eng. Sci.* **2023**, *270*, 118515. [CrossRef]
14. Barkanyi, A.; Chovan, T.; Nemeth, S.; Abonyi, J. Modelling for Digital Twins—Potential Role of Surrogate Models. *Processes* **2021**, *9*, 476. [CrossRef]

15. Mencarelli, L.; Pagot, A.; Duchêne, P. Surrogate-Based Modeling Techniques with Application to Catalytic Reforming and Isomerization Processes. *Comput. Chem. Eng.* **2020**, *135*, 106772. [CrossRef]
16. Quirante, N.; Javaloyes, J.; Caballero, J. Rigorous Design of Distillation Columns Using Surrogate Models Based on Kriging Interpolation. *AIChE J.* **2015**, *61*, 2169–2187. [CrossRef]
17. Kudela, J.; Matousek, R. Recent Advances and Applications of Surrogate Models for Finite Element Method Computations: A Review. *Soft Comput.* **2022**, *26*, 13709–13733. [CrossRef]
18. Ramancha, M.; Vega, M.; Conte, J.; Todd, M.; Hu, Z. Bayesian Model Updating with Finite Element vs Surrogate Models: Application to a Miter Gate Structural System. *Eng. Struct.* **2022**, *272*, 114901. [CrossRef]
19. Kim, S.; Boukouvala, F. Machine Learning-Based Surrogate Modeling for Data-Driven Optimization: A Comparison of Subset Selection for Regression Techniques. *Optim. Lett.* **2020**, *14*, 989–1010. [CrossRef]
20. Smola, A.; Vishwanathan, S. *Introduction to Machine Learning*; Cambridge University: Cambridge, UK, 2008; Volume 32, p. 34.
21. Badillo, S.; Banfai, B.; Birzele, F.; Davydov, I.; Hutchinson, L.; Kam-Thong, T.; Siebourg-Polster, J.; Steiert, B.; Zhang, J. An Introduction to Machine Learning. *Clin. Pharmacol. Ther.* **2020**, *107*, 871–885. [CrossRef]
22. Alpaydin, E. *Introduction to Machine Learning*; MIT Press: Cambridge, MA, USA, 2020.
23. Baştanlar, Y.; Özuysal, M. Introduction to Machine Learning. In *miRNomics: MicroRNA Biology and Computational Analysis*; Springer: Berlin, Germany, 2014; pp. 105–128.
24. Nasteski, V. An Overview of the Supervised Machine Learning Methods. *Horizons B* **2017**, *4*, 51–62. [CrossRef]
25. Shenfield, A.; Howarth, M. A Novel Deep Learning Model for the Detection and Identification of Rolling Element-Bearing Faults. *Sensors* **2020**, *20*, 5112. [CrossRef]
26. Raschka, S.; Patterson, J.; Nolet, C. Machine Learning in Python: Main Developments and Technology Trends in Data Science, Machine Learning, and Artificial Intelligence. *Information* **2020**, *11*, 193. [CrossRef]
27. Vapnik, V. *Statistical Learning Theory*; Wiley: New York, NY, USA, 1998.
28. Astray, G.; Mejuto, J.; Martínez-Martínez, V.; Nevares, I.; Alamo-Sanza, M.; Simal-Gandara, J. Prediction Models to Control Aging Time in Red Wine. *Molecules* **2019**, *24*, 826. [CrossRef]
29. Qu, C.; Wang, Z.; Jin, X.; Wang, X.; Wang, D. A moisture content prediction model for deep bed peanut drying using support vector regression. *J. Food Process Eng.* **2020**, *43*, e13510. [CrossRef]
30. Sultana, N.; Hossain, S.Z.; Abusaad, M.; Alanbar, N.; Senan, Y.; Razzak, S. Prediction of biodiesel production from microalgal oil using Bayesian optimization algorithm-based machine learning approaches. *Fuel* **2022**, *309*, 122184. [CrossRef]
31. MacKay, D. *Information Theory, Inference, and Learning Algorithms*; Cambridge University Press: Cambridge, UK, 2003.
32. Forrester, A.; Sobester, A.; Keane, A. *Engineering Design via Surrogate Modelling: A Practical Guide*; John Wiley & Sons: Chichester, UK, 2008.
33. Chakraborty, S.; Adhikari, S.; Ganguli, R. The Role of Surrogate Models in the Development of Digital Twins of Dynamic Systems. *Appl. Math. Model.* **2021**, *90*, 662–681. [CrossRef]
34. Malvandi, A.; Feng, H.; Kamruzzaman, M. Application of NIR spectroscopy and multivariate analysis for Non-destructive evaluation of apple moisture content during ultrasonic drying. *Spectrochim. Acta Part A Mol. Biomol. Spectrosc.* **2022**, *269*, 120733. [CrossRef] [PubMed]
35. Bhonsale, S.; Mores, W.; Van Impe, J. Dynamic optimisation of beer fermentation under parametric uncertainty. *Fermentation* **2021**, *7*, 285. [CrossRef]
36. Seratlic, S.; Guha, B.; Moore, S. Advances in Spectroscopic Methods for Predicting Cheddar Cheese Maturity: A Review of FT-IR, NIR, and NMR Techniques. *NDT* **2024**, *2*, 392–416. [CrossRef]
37. Zhang, Z.; Xiao, D.; Choi, K.S.; Mao, X. The fusion of flow field data with multiple fidelities. *Phys. Fluids* **2022**, *34*, 097113. [CrossRef]
38. Liu, H.; Ong, Y.S.; Shen, X.; Cai, J. When Gaussian process meets big data: A review of scalable GPs. *IEEE Trans. Neural Netw. Learn. Syst.* **2020**, *31*, 4405–4423. [CrossRef] [PubMed]
39. Livingstone, D. *Artificial Neural Networks: Methods and Applications*; Springer: Berlin, Germany, 2008; Volume 458.
40. Abraham, A. *Artificial Neural Networks*; John Wiley & Sons, Ltd.: Chichester, UK, 2005.
41. Ding, H.; Hou, H.; Wang, L.; Cui, X.; Yu, W.; Wilson, D.I. Application of convolutional neural networks and recurrent neural networks in food safety. *Foods* **2025**, *14*, 247. [CrossRef]
42. Zatsu, V.; Shine, A.; Tharakan, J.; Peter, D.; Ranganathan, T.; Alotaibi, S.; Mugabi, R.; Muhsinah, A.; Waseem, M.; Nayik, G. Revolutionizing the Food Industry: The Transformative Power of Artificial Intelligence—A Review. *Food Chem. X* **2024**, *24*, 101867. [CrossRef]
43. Rodríguez, J.; Hamzaoui, Y.; Hernández, J.; García, J.; Flores, J.; Tejeda, A. The Use of Artificial Neural Network (ANN) for Modeling the Useful Life of the Failure Assessment in Blades of Steam Turbines. *Eng. Fail. Anal.* **2013**, *35*, 562–575. [CrossRef]
44. Khan, M.I.H.; Sablani, S.S.; Joardder, M.; Karim, M. Application of machine learning-based approach in food drying: Opportunities and challenges. *Dry. Technol.* **2022**, *40*, 1051–1067. [CrossRef]

45. Islam, M.R.; Zamil, M.Z.H.; Rayed, M.E.; Kabir, M.M.; Mridha, M.; Nishimura, S.; Shin, J. Deep learning and computer vision techniques for enhanced quality control in manufacturing processes. *IEEE Access* **2024**, *12*, 121449–121479 . [CrossRef]
46. Bhagya Raj, G.; Dash, K.K. Comprehensive study on applications of artificial neural network in food process modeling. *Crit. Rev. Food Sci. Nutr.* **2022**, *62*, 2756–2783. [CrossRef]
47. Llacay, B.; Peffer, G. Categorical Surrogation of Agent-Based Models: A Comparative Study of Machine Learning Classifiers. *Expert Syst.* **2023**, *42*, e13342. [CrossRef]
48. Shan, S.; Wang, G. Survey of Modeling and Optimization Strategies to Solve High-Dimensional Design Problems with Computationally-Expensive Black-Box Functions. *Struct. Multidiscip. Optim.* **2010**, *41*, 219–241. [CrossRef]
49. Misener, R.; Biegler, L. Formulating Data-Driven Surrogate Models for Process Optimization. *Comput. Chem. Eng.* **2023**, *179*, 108411. [CrossRef]
50. Zhai, J.; Boukouvala, F. Data-Driven Spatial Branch-and-Bound Algorithms for Box-Constrained Simulation-Based Optimization. *J. Glob. Optim.* **2022**, *82*, 21–50. [CrossRef]
51. Cuomo, S.; Di Cola, V.; Giampaolo, F.; Rozza, G.; Raissi, M.; Piccialli, F. Scientific Machine Learning through Physics-Informed Neural Networks: Where We Are and What's Next. *J. Sci. Comput.* **2022**, *92*, 88. [CrossRef]
52. Karniadakis, G.; Kevrekidis, I.; Lu, L.; Perdikaris, P.; Wang, S.; Yang, L. Physics-Informed Machine Learning. *Nat. Rev. Phys.* **2021**, *3*, 422–440. [CrossRef]
53. Raissi, M.; Perdikaris, P.; Karniadakis, G.E. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *J. Comput. Phys.* **2019**, *378*, 686–707. [CrossRef]
54. Huang, B.; Wang, J. Applications of Physics-Informed Neural Networks in Power Systems—A Review. *IEEE Trans. Power Syst.* **2022**, *38*, 572–588. [CrossRef]
55. Purlis, E. Physics-Informed Machine Learning: The Next Big Trend in Food Process Modelling? *Curr. Food Sci. Technol. Rep.* **2024**, *2*, 1–6. [CrossRef]
56. Chen, X.; Chen, R.; Wan, Q.; Xu, R.; Liu, J. An Improved Data-Free Surrogate Model for Solving Partial Differential Equations Using Deep Neural Networks. *Sci. Rep.* **2021**, *11*, 19507. [CrossRef] [PubMed]
57. Cai, S.; Mao, Z.; Wang, Z.; Yin, M.; Karniadakis, G. Physics-Informed Neural Networks (PINNs) for Fluid Mechanics: A Review. *Acta Mech. Sin.* **2021**, *37*, 1727–1738. [CrossRef]
58. Singh, P.; Pandey, S.; Manik, S. A comprehensive review of the dairy pasteurization process using machine learning models. *Food Control* **2024**, *164*, 110574. [CrossRef]
59. Khan, M.I.H.; Batuwatta-Gamage, C.P.; Karim, M.; Gu, Y. Fundamental understanding of heat and mass transfer processes for physics-informed machine learning-based drying modelling. *Energies* **2022**, *15*, 9347. [CrossRef]
60. Vinestock, T.; Short, M.; Ward, K.; Guo, M. Computer-aided chemical engineering research advances in precision fermentation. *Curr. Opin. Food Sci.* **2024**, *58*, 101196. [CrossRef]
61. Li, Y.; Wang, Y.; Yan, L. Surrogate Modeling for Bayesian Inverse Problems Based on Physics-Informed Neural Networks. *J. Comput. Phys.* **2023**, *475*, 111841. [CrossRef]
62. Würth, T.; Krauß, C.; Zimmerling, C.; Kärger, L. Physics-Informed Neural Networks for Data-Free Surrogate Modelling and Engineering Optimization—An Example from Composite Manufacturing. *Mater. Des.* **2023**, *231*, 112034. [CrossRef]
63. Wang, J.; Xiao, X.; Feng, X.; Xu, H. An improved physics-informed neural network with adaptive weighting and mixed differentiation for solving the incompressible Navier–Stokes equations. *Nonlinear Dyn.* **2024**, *112*, 16113–16134. [CrossRef]
64. Chen, W.; Howard, A.A.; Stinis, P. Self-adaptive weights based on balanced residual decay rate for physics-informed neural networks and deep operator networks. *J. Comput. Phys.* **2025**, 114226. [CrossRef]
65. Perez, S.; Maddu, S.; Sbalzarini, I.F.; Poncet, P. Adaptive weighting of Bayesian physics informed neural networks for multitask and multiscale forward and inverse problems. *J. Comput. Phys.* **2023**, *491*, 112342. [CrossRef]
66. Nayak, J.; Vakula, K.; Dinesh, P.; Naik, B.; Pelusi, D. Intelligent food processing: Journey from artificial neural network to deep learning. *Comput. Sci. Rev.* **2020**, *38*, 100297. [CrossRef]
67. Liu, Y.; Pu, H.; Sun, D.W. Efficient extraction of deep image features using convolutional neural network (CNN) for applications in detecting and analysing complex food matrices. *Trends Food Sci. Technol.* **2021**, *113*, 193–204. [CrossRef]
68. Özsert Yiğit, G.; Özyildirim, B.M. Comparison of convolutional neural network models for food image classification. *J. Inf. Telecommun.* **2018**, *2*, 347–357. [CrossRef]
69. Luo, N.; Xu, D.; Xing, B.; Yang, X.; Sun, C. Principles and applications of convolutional neural network for spectral analysis in food quality evaluation: A review. *J. Food Compos. Anal.* **2024**, *128*, 105996. [CrossRef]
70. Chakravartula, S.S.N.; Moscetti, R.; Bedini, G.; Nardella, M.; Massantini, R. Use of convolutional neural network (CNN) combined with FT-NIR spectroscopy to predict food adulteration: A case study on coffee. *Food Control* **2022**, *135*, 108816. [CrossRef]
71. Addanki, M.; Patra, P.; Kandra, P. Recent advances and applications of artificial intelligence and related technologies in the food industry. *Appl. Food Res.* **2022**, *2*, 100126. [CrossRef]

72. Bahaghighat, M.; Abedini, F.; S'hoyan, M.; Molnar, A.J. Vision inspection of bottle caps in drink factories using convolutional neural networks. In Proceedings of the 2019 IEEE 15th International Conference on Intelligent Computer Communication and Processing (ICCP), Cluj-Napoca, Romania, 5–7 September 2019 ; IEEE: Piscataway, NJ, USA, 2019; pp. 381–385.
73. Tarwani, K.M.; Edem, S. Survey on recurrent neural network in natural language processing. *Int. J. Eng. Trends Technol.* **2017**, *48*, 301–304. [CrossRef]
74. Chung, J.; Gulcehre, C.; Cho, K.; Bengio, Y. Gated feedback recurrent neural networks. In Proceedings of the International Conference on Machine Learning, PMLR, 2015, Lile, France, 6–11 July 2015; pp. 2067–2075.
75. Zargar, S. *Introduction to Sequence Learning Models: RNN, LSTM, GRU*; Department of Mechanical and Aerospace Engineering, North Carolina State University: Raleigh, NC, USA, 2021.
76. Kim, S.Y.; Park, S.; Hong, S.J.; Kim, E.; Nurhisna, N.I.; Park, J.; Kim, G. Time-series prediction of onion quality changes in cold storage based on long short-term memory networks. *Postharvest Biol. Technol.* **2024**, *213*, 112927. [CrossRef]
77. Weerakody, P.B.; Wong, K.W.; Wang, G.; Ela, W. A review of irregular time series data handling with gated recurrent neural networks. *Neurocomputing* **2021**, *441*, 161–178. [CrossRef]
78. Wahid, A.; Breslin, J.G.; Intizar, M.A. Prediction of machine failure in industry 4.0: A hybrid CNN-LSTM framework. *Appl. Sci.* **2022**, *12*, 4221. [CrossRef]
79. Khan, P.W.; Byun, Y.C.; Park, N. IoT-blockchain enabled optimized provenance system for food industry 4.0 using advanced deep learning. *Sensors* **2020**, *20*, 2990. [CrossRef]
80. Matla, Y.; Yannamaneni, R.R.; Pappas, G. Globalizing Food Items Based on Ingredient Consumption. *Sustainability* **2024**, *16*, 7524. [CrossRef]
81. Bowler, A.; Rodgers, S.; Cook, D.; Watson, N. Bayesian and Ultrasonic Sensor Aided Multi-Objective Optimisation for Sustainable Clean-in-Place Processes. *Food Bioprod. Process.* **2023**, *141*, 23–35. [CrossRef]
82. Datta, A.; Nicolaï, B.; Vitrac, O.; Verboven, P.; Erdogdu, F.; Marra, F.; Sarghini, F.; Koh, C. Computer-Aided Food Engineering. *Nat. Food* **2022**, *3*, 894–904. [CrossRef] [PubMed]
83. Di Martino, M.; Avraamidou, S.; Cook, J.; Pistikopoulos, E. An Optimization Framework for the Design of Reverse Osmosis Desalination Plants under Food-Energy-Water Nexus Considerations. *Desalination* **2021**, *503*, 114937. [CrossRef]
84. Chiu, M.C.; Yan, W.M.; Bhat, S.; Huang, N.F. Development of Smart Aquaculture Farm Management System Using IoT and AI-Based Surrogate Models. *J. Agric. Food Res.* **2022**, *9*, 100357. [CrossRef]
85. Khan, M.; Moallemi, E.; Thiruvady, D.; Nazari, A.; Bryan, B. Machine Learning-Based Surrogate Modelling of a Robust, Sustainable Development Goal (SDG)-Compliant Land-Use Future for Australia at High Spatial Resolution. *J. Environ. Manag.* **2024**, *363*, 121296. [CrossRef]
86. Datta, A. Status of Physics-Based Models in the Design of Food Products, Processes, and Equipment. *Compr. Rev. Food Sci. Food Saf.* **2008**, *7*, 121–129. [CrossRef]
87. Fisher, O.; Watson, N.; Escrig, J.; Witt, R.; Porcu, L.; Bacon, D.; Rigley, M.; Gomes, R. Considerations, Challenges and Opportunities When Developing Data-Driven Models for Process Manufacturing Systems. *Comput. Chem. Eng.* **2020**, *140*, 106881. [CrossRef]
88. Nkosi, N.; Tumba, K. Optimization and Energy Assessment of Carbon Dioxide Hydrate-Based Fruit Juice Concentration Process. *Food Bioproc. Technol.* **2024**, *17*, 1845–1861. [CrossRef]
89. Awuah, G.; Ramaswamy, H.; Economides, A. Thermal Processing and Quality: Principles and Overview. *Chem. Eng. Process. Process Intensif.* **2007**, *46*, 584–602. [CrossRef]
90. Kumar, I.; Rawat, J.; Mohd, N.; Husain, S. Opportunities of Artificial Intelligence and Machine Learning in the Food Industry. *J. Food Qual.* **2021**, *2021*, 4535567. [CrossRef]
91. Becker, D.; Schmitt, C.; Bovetto, L.; Rauh, C.; McHardy, C.; Hartmann, C. Optimization of Complex Food Formulations Using Robotics and Active Learning. *Innov. Food Sci. Emerg. Technol.* **2023**, *83*, 103232. [CrossRef]
92. Ladha-Sabur, A.; Bakalis, S.; Fryer, P.; Lopez-Quiroga, E. Mapping Energy Consumption in Food Manufacturing. *Trends Food Sci. Technol.* **2019**, *86*, 270–280. [CrossRef]
93. Naresh Kumar, S.; Chakabarti, B. Energy and Carbon Footprint of Food Industry. In *Energy Footprints of the Food and Textile Sectors*; Springer: Cham, Switzerland, 2019; pp. 19–44.
94. Corigliano, O.; Algieri, A. A Comprehensive Investigation on Energy Consumptions, Impacts, and Challenges of the Food Industry. *Energy Convers. Manag. X* **2024**, *23*, 100661. [CrossRef]
95. Meyers, S.; Schmitt, B.; Chester-Jones, M.; Sturm, B. Energy Efficiency, Carbon Emissions, and Measures towards Their Improvement in the Food and Beverage Sector for Six European Countries. *Energy* **2016**, *104*, 266–283. [CrossRef]
96. Millán, G.; Llano, E.; Globisch, J.; Durand, A.; Hettesheimer, T.; Alcalde, E. Increasing Energy Efficiency in the Food and Beverage Industry: A Human-Centered Design Approach. *Sustainability* **2020**, *12*, 7037. [CrossRef]
97. Clairand, J.M.; Briceno-Leon, M.; Escriva-Escriva, G.; Pantaleo, A. Review of Energy Efficiency Technologies in the Food Industry: Trends, Barriers, and Opportunities. *IEEE Access* **2020**, *8*, 48015–48029. [CrossRef]

98. Durkin, A.; Otte, L.; Guo, M. Surrogate-Based Optimisation of Process Systems to Recover Resources from Wastewater. *Comput. Chem. Eng.* **2024**, *182*, 108584. [CrossRef]
99. Xiong, Z.; Guo, K.; Cai, H.; Liu, H.; Xiang, W.; Liu, C. Distillation Process Optimization: A Screening-Clustering Assisted Kriging Optimization Method. *Chem. Eng. Sci.* **2021**, *238*, 116597. [CrossRef]
100. Hüllen, G.; Zhai, J.; Kim, S.; Sinha, A.; Realff, M.; Boukouvala, F. Managing Uncertainty in Data-Driven Simulation-Based Optimization. *Comput. Chem. Eng.* **2020**, *136*, 106519. [CrossRef]
101. Yondo, R.; Andrés, E.; Valero, E. A Review of Design of Experiments and Surrogate Models in Aircraft Real-Time and Many-Query Aerodynamic Analyses. *Prog. Aerosp. Sci.* **2018**, *96*, 23–61. [CrossRef]
102. Wang, C.; Duan, Q.; Gong, W.; Ye, A.; Di, Z.; Miao, C. An Evaluation of Adaptive Surrogate Modeling Based Optimization with Two Benchmark Problems. *Environ. Model. Softw.* **2014**, *60*, 167–179. [CrossRef]
103. Dhal, S.B.; Kar, D. Leveraging artificial intelligence and advanced food processing techniques for enhanced food safety, quality, and security: A comprehensive review. *Discov. Appl. Sci.* **2025**, *7*, 75. [CrossRef]
104. Vaswani, A.; Shazeer, N.; Parmar, N.; Uszkoreit, J.; Jones, L.; Gomez, A.N.; Kaiser, Ł.; Polosukhin, I. Attention is all you need. *Adv. Neural Inf. Process. Syst.* **2017**, *30* .
105. Gim, M.; Park, D.; Spranger, M.; Maruyama, K.; Kang, J. Recipebowl: A cooking recommender for ingredients and recipes using set transformer. *IEEE Access* **2021**, *9*, 143623–143633. [CrossRef]
106. Zhao, S.; Bai, Z.; Wang, S.; Gu, Y. Research on automatic classification and detection of mutton multi-parts based on swin-transformer. *Foods* **2023**, *12*, 1642. [CrossRef]