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Mathematical modelling in food processing: Overview

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Abstract

Mathematical modelling plays a vital role in understanding and optimizing various aspects of food processing. This review paper aims to provide an overview of the applications of mathematical modelling and equations in the field of food processing. It explores the diverse areas of food processing where mathematical models have been successfully employed, highlighting their benefits and challenges. Additionally, it discusses the significance of mathematical modelling in enhancing food safety, quality, and efficiency. This review serves as a valuable resource for researchers, engineers, and professionals involved in the food processing industry.

Keywords: Mathematical modelling, equations, food processing

Introduction

Food processing is a diverse field encompassing various operations like heating, cooling, mixing, drying, and packaging, all of which require a deep understanding of the underlying physical, chemical, and biological processes^[1]. Mathematical modelling has emerged as a valuable tool in this context, enabling the analysis, optimization, and prediction of these intricate processes. Mathematical modelling involves the formulation of mathematical equations based on fundamental principles and empirical data to describe and simulate real-world phenomena^[2]. In food processing, mathematical models have been extensively utilized to gain insights into heat transfer, mass transfer, fluid flow, reaction kinetics, and microbial growth. These models provide a systematic framework for analyzing and optimizing process parameters, predicting product quality and safety, and facilitating decision-making across the food processing chain^[3].

Mathematical modelling also plays a significant role in food safety through predictive microbiology. Additionally, mathematical models aid in estimating shelf-life, assisting manufacturers in optimizing storage conditions and packaging techniques to extend product freshness while minimizing waste^[4]. Mathematical modelling proves beneficial in resource and energy optimization. By analyzing the interplay between process parameters and resource utilization, mathematical models assist in minimizing energy consumption, reducing waste generation, and optimizing production efficiency^[5]. This contributes to the implementation of sustainable and environmentally friendly practices within the food processing industry. Mathematical modelling also presents challenges such as data availability, accuracy, model validation, and computational complexities^[6]. However, ongoing advancements in computational methods, data-driven modelling, and the integration of machine learning techniques offer opportunities to overcome these challenges and further enhance the application of mathematical modelling in the field.

Types of mathematical models

Mathematical models can be broadly classified into different types based on their characteristics and the nature of the phenomena they represent. Some common types of mathematical models are detailed in Table.1.

Table 1: Types of mathematical models in food processing

Type of model	Description	References
Empirical Models	Empirical models are based on experimental observations and data. They describe the relationship between variables without explicitly considering the underlying physical or mechanistic principles. Empirical models are often used when the underlying mechanisms are not well understood or when precise mathematical equations are difficult to establish.	[1, 3, 5]
Mechanistic Models	Mechanistic models are based on fundamental principles and physical laws governing the system being modelled. These models use mathematical equations to represent the relationships between variables and simulate the behaviour of the system.	[1, 6]
Deterministic Models	Deterministic models assume that the future behaviour of the system can be precisely determined given the initial conditions and parameters of the model. These models use a set of mathematical equations to represent the relationships between variables and provide a deterministic prediction of system behaviour over time.	[7, 8]
Stochastic Models	Stochastic models incorporate randomness or uncertainty into the model's parameters or initial conditions. These models take into account the probabilistic nature of the system and use techniques such as probability distributions or Monte Carlo simulations to estimate the range of possible outcomes.	[7, 9]
Statistical Models	Statistical models are used to analyze and describe relationships between variables based on observed data. Statistical models are commonly used in data analysis, regression analysis, and hypothesis testing.	[10, 11]
Optimization Models	Optimization models are used to determine the optimal values of decision variables that maximize or minimize an objective function while satisfying a set of constraints. These models help in optimizing process parameters, resource allocation, or system design. Optimization models use mathematical techniques such as linear programming, nonlinear programming, or integer programming.	[12]
Simulation Models	Simulation models are used to replicate the behaviour of a real-world system by creating a computer-based model. These models incorporate mathematical equations and algorithms to simulate the processes, interactions, and dynamics of the system over time. Simulation models are often used to study complex systems, evaluate different scenarios, and understand the implications of various decisions.	[10, 13]

Depending on the specific application and research objectives, researchers may utilize a combination of these models or develop customized models that suit their needs.

Parameters and variables used in food processing models:

Food processing models involve various parameters and variables that represent the characteristics, conditions, and properties of the food system being studied. Common parameters and variables used in food processing models are detailed in Table 2 below.

Table 2: Parameters and variables used in food processing models

Parameters and variables		
Time: It influences the duration of processing operations, microbial growth, and quality changes. Temperature: It affects heat transfer, microbial growth, enzyme activity, and chemical reactions. [1, 3, 5]	Physical Properties: These properties influence the behaviour of the food system, such as flow characteristics, heat transfer rates, and mass transfer rates [1, 3, 5]	Moisture Content: It affects product quality, microbial stability, and texture. Moisture content can be represented as a variable or a parameter that changes during the processing operation. [1, 3, 5]
pH: It is a measure of acidity or alkalinity and its impact on microbial growth, enzyme activity, and chemical reactions in food processing that involve fermentation, preservation, and other pH-dependent processes. [13, 14]	Mass and Volume: These parameters are important for calculating mass balances, mixing ratios, and determining the composition of the final product. [15]	Concentration: It is commonly used in models related to the extraction, diffusion, and concentration processes. Concentration can be represented as a variable that changes over time or space. [15, 16]
Heat Transfer Coefficients: These coefficients depend on factors such as surface area, thermal conductivity, and flow conditions. They are essential parameters in heat transfer models for processes like thermal pasteurization, blanching, and sterilization. [17]	Reaction Rates: Represented as variables or parameters in kinetic models for processes like enzymatic reactions, Maillard browning, and lipid oxidation. [16, 17]	Microbial Parameters: It is associated with microbial growth, survival, and inactivation are crucial. These may include parameters like microbial growth rates, lag times, activation energies, and death rates. [18]

The specific parameters and variables employed depend on the nature of the process being modelled and the research

objectives. Table 3 depicts some mathematical modelling in food processing.

Table 3: Mathematical modelling in food processing [18 -21, 23, 25]

Mode	Area	Type of models
Heat Transfer	Applications of heat transfer models in thermal processing	Fourier's Law Model, Newton's Law of Cooling, Stefan-Boltzmann Law, Heat Exchanger Models, Computational Fluid Dynamics (CFD) Models, Finite Element Method (FEM) Models and Analytical and Empirical Models
	Heat conduction, convection, and radiation equations	
	Modelling heat transfer in food drying, baking, and pasteurization	
Mass Transfer	Diffusion and Fick's laws in modelling mass transfer	Fick's Law Model, Stefan-Maxwell Model, Convective Mass Transfer Models, Mass Transfer in Porous Media, Mass Transfer in Chemical Reaction Models, Computational Fluid Dynamics (CFD) Models, Empirical and Semi-Empirical Models.
	Applications of mass transfer models in food drying, freezing, and extraction processes	
Fluid Flow	Equations for fluid flow in pipes, channels, and porous media	Eulerian Model, Reynolds-Averaged Navier-Stokes (RANS) Model, Large Eddy Simulation (LES), Direct Numerical Simulation (DNS), Lattice Boltzmann Method (LBM), Boundary Element Method (BEM), Analytical Models
	Modelling fluid flow in food processing operations such as mixing, pumping, and filtration.	
Reaction Kinetics	Chemical reaction equations and rate constants	Elementary Reaction Models, Rate Laws, Arrhenius Equation, Reaction Mechanism Models, Enzyme Kinetics Models, Homogeneous and Heterogeneous Reaction Models, Computational Reaction Kinetics Models
	Modelling enzymatic reactions, microbial growth, and shelf-life prediction	

Mathematical modelling in common unit operations

Mathematical models play a crucial role in the analysis, design, and optimization of various unit operations in food processing and other related fields. These models provide

mathematical representations of the underlying physical processes and help in predicting the behaviour of unit operations ^[20, 21, 23], (Table 4).

Table 4: Examples of mathematical models used in common unit operations

Unit Operations	Mathematical Models	Process
Distillation	Equilibrium Stage Models	These models divide the distillation column into theoretical equilibrium stages and describe the mass and heat transfer between the vapour and liquid phases at each stage. The models include material and energy balances, as well as vapour-liquid equilibrium relationships.
	Rigorous Tray-to-Tray Models	These models simulate the distillation column as a series of trays or stages and include detailed mass and energy balances, tray efficiencies, and pressure drop calculations.
Heat Exchangers	LMTD (Log Mean Temperature Difference) Method	This method is used to calculate the heat transfer rate in a heat exchanger with a parallel flow, counterflow, or cross-flow arrangement. It is based on the assumption of a constant overall heat transfer coefficient and a constant heat capacity rate.
	Effectiveness-NTU (Number of Transfer Units) Method	This method is applicable to heat exchangers with complex flow patterns or non-uniform temperature profiles. It relates the heat transfer effectiveness to the number of transfer units, which represents the heat capacity rate ratio of the two fluid streams.
Filtration	Cake Filtration Models	These models describe the filtration of a suspension through a porous medium, such as a filter cake or filter media. They consider variables such as cake thickness, cake resistance, pressure drop, and filtration rate, incorporating equations such as Darcy's law and filtration resistance equations.
	Filtration Efficiency Models	These models quantify the separation efficiency of a filtration process based on particle size distribution, filtration medium characteristics, and operating parameters. They help estimate the removal efficiency and predict the filtration performance.
Fluid Flow	Bernoulli's Equation	Bernoulli's equation is used to describe the relationship between fluid pressure, velocity, and elevation along a streamline. It is applicable to incompressible flow and is commonly used in piping systems, pump calculations, and flow measurements.
	Navier-Stokes Equations	The Navier-Stokes equations represent the fundamental equations of fluid motion and describe the conservation of mass, momentum, and energy. These equations, along with appropriate boundary conditions and simplifying assumptions, are used in computational fluid dynamics (CFD) simulations to analyze complex fluid flow phenomena.
Mixing	Perfectly Mixed Model	This model assumes complete mixing and uniform composition throughout the mixing vessel or reactor. It is commonly used for well-agitated systems where the mixing time is significantly shorter than the reaction time.
	Residence Time Distribution (RTD) Models	RTD models characterize the distribution of residence times of fluid elements in a mixing system. These models, such as the ideal stirred tank reactor (CSTR) model or the plug flow reactor (PFR) model, provide insights into the extent of mixing and the flow behaviour within the system.
Crystallization	Population Balance Models	These models describe the crystal size distribution in a crystallization process. They incorporate the rates of nucleation, growth, agglomeration, and breakage of crystals, as well as mass and energy balances, to predict the crystal size distribution and overall process performance.

Predictive Microbiology and Food Safety

1. Use of mathematical models to predict microbial growth and inactivation: Mathematical models play a crucial role in predicting microbial growth and

inactivation in food processing. These models provide valuable insights into the behaviour of microorganisms under different environmental conditions and help assess the effectiveness of control measures. (Table 5)

Table 5: Approaches and mathematical models are used to predict microbial growth and inactivation

Primary Models ^[20-27]	
Growth Models	Primary models describe the growth rate of microorganisms as a function of environmental factors such as temperature, pH, and water activity. Examples include the exponential, logistic, and Gompertz models. These models assume that growth is only influenced by intrinsic factors and do not consider the effects of external stresses or inhibitory factors.
Inactivation Models	Primary models for microbial inactivation describe the decline in microbial populations over time or with exposure to a lethal agent, such as heat or antimicrobial treatments. Examples include the first-order, Weibull, and biphasic models. These models assume a single population of microorganisms and do not account for factors like microbial subpopulations or adaptive responses.
Secondary Models	Secondary models build upon primary models by incorporating additional factors that influence microbial growth or inactivation. These factors may include the presence of inhibitory compounds, competitive microorganisms, or stressors such as high pressure or UV radiation. Secondary models aim to improve the accuracy and applicability of predictions by considering more complex scenarios and environmental conditions.
Response Surface Models	Response surface models (RSM) allow the simultaneous evaluation of multiple environmental factors on microbial growth or inactivation. RSM uses statistical techniques to determine the optimal combination of factors that minimizes or maximizes microbial populations. This approach is particularly useful for process optimization and designing control strategies.
Predictive Microbiology Software	Predictive microbiology software packages, such as ComBase and USDA Pathogen Modeling Program (PMP), incorporate various mathematical models and databases to predict microbial growth, inactivation, and the effects of different environmental conditions. These tools provide user-friendly interfaces and enable researchers and food processors to simulate and predict microbial behaviour in specific food systems

2. Risk assessment and decision-making in food safety:
 Risk assessment plays a crucial role in food safety by providing a systematic and science-based approach to

identifying, evaluating, and managing potential hazards associated with food products and processes [23-26]. (Table. 6).

Table 6: Key steps and considerations in risk assessment and decision-making in food safety

Hazard Identification	The first step in risk assessment is to identify and characterize potential hazards that may be present in the food system. This includes biological hazards (e.g., pathogens, toxins), chemical hazards (e.g., pesticides, allergens), and physical hazards (e.g., foreign objects). Comprehensive knowledge of potential hazards is essential for risk assessment and subsequent risk management strategies.
Exposure Assessment	Exposure assessment involves estimating the likelihood and level of exposure to hazards by considering various factors such as consumption patterns, processing methods, storage conditions, and consumer behaviour. It helps determine the potential health risks associated with specific hazards and identifies vulnerable populations that may be at higher risk.
Hazard Characterization	Hazard characterization involves evaluating the severity of adverse health effects associated with exposure to specific hazards. This step includes understanding the dose-response relationship, toxicological data, and epidemiological studies to assess the potential health impacts on consumers.
Risk Characterization	Risk characterization integrates hazard identification, exposure assessment, and hazard characterization to quantify and communicate the overall risk to public health. This step involves estimating the likelihood and severity of adverse health effects resulting from exposure to specific hazards. Risk characterization helps prioritize risks, set safety standards, and establish risk management strategies.
Risk Management	Risk management involves the development and implementation of strategies to control or mitigate identified risks. It includes regulatory measures, industry practices, quality assurance programs, and other interventions to reduce or eliminate hazards. Risk management decisions are based on risk assessment outcomes, societal values, and risk-benefit considerations
Risk Communication	Effective risk communication is crucial for the transparent and timely dissemination of risk information to various stakeholders, including consumers, industry, regulatory agencies, and policymakers. It involves conveying complex scientific information in a clear and understandable manner to facilitate informed decision-making and foster trust
Monitoring and Surveillance	Ongoing monitoring and surveillance are essential for assessing the effectiveness of risk management measures, detecting emerging risks, and evaluating changes in food safety practices. Data from surveillance systems, outbreak investigations, and laboratory analyses provide valuable insights to update risk assessments and guide decision-making.

Challenges and Future Perspectives

Challenges

- 1. Data Availability and Quality:** One of the significant challenges in risk assessment and decision-making in food safety is the availability and quality of data. Accurate and comprehensive data on hazards, exposure levels, and health effects are crucial for robust risk assessments. However, data may be limited, incomplete, or subject to variability, making it challenging to accurately quantify risks and make informed decisions.
- 2. Emerging Hazards and Complex Systems:** The food industry is dynamic, with the emergence of new hazards and complex production systems. Identifying and assessing risks associated with emerging hazards, such as new pathogens or novel processing techniques, can be challenging. Understanding the interactions between different hazards, their cumulative effects, and the impact of processing conditions adds complexity to risk assessment.
- 3. Uncertainty and Variability:** Risk assessments involve dealing with uncertainty and variability, both inherent in the data and the modelling process. Uncertainty arises from gaps in knowledge, limitations in data quality, and assumptions made during the risk assessment process. Addressing uncertainty and variability requires advanced statistical methods and sensitivity analysis to assess their impact on risk estimates and decision-making.
- 4. Globalization and Supply Chains:** With the globalization of the food supply chain, risks can originate from various sources and traverse multiple countries. This complexity poses challenges in risk assessment and management, as coordinating efforts across jurisdictions and ensuring harmonized approaches becomes critical.

epidemiological data, can improve risk assessments. The integration of real-time monitoring systems, advanced analytics, and emerging technologies like blockchain can enhance data quality, traceability, and rapid response to food safety issues.

- 2. Predictive Analytics and Modeling:** The use of advanced predictive analytics and modelling techniques, including machine learning and artificial intelligence, can improve risk assessments. These techniques can analyze large datasets, identify patterns, and predict potential risks, allowing for proactive risk management strategies.
- 3. One Health Approach:** Adopting a One Health approach that integrates human, animal, and environmental health can enhance the understanding of complex foodborne disease dynamics. This approach considers the interconnectedness of the food chain, zoonotic diseases, and environmental factors, leading to more comprehensive risk assessments.
- 4. Rapid Diagnostics and Surveillance:** Advancements in rapid diagnostic technologies and real-time surveillance systems can enable early detection and response to foodborne hazards. These technologies, including DNA-based methods and sensor technologies, can improve the speed and accuracy of identifying hazards, enabling targeted risk management interventions.
- 5. Stakeholder Collaboration and Risk Communication:** Enhancing collaboration and communication between stakeholders, including government agencies, industry, academia, and consumers, is crucial for effective risk assessment and management. Clear and transparent risk communication, tailored to different audiences, fosters trust, improves compliance, and empowers consumers to make informed choices.

Future Perspectives

- 1. Advanced Data Collection and Integration:** Enhancing data collection systems and integrating diverse data sources, including genomics, metagenomics, and

Conclusion

Mathematical modelling and equations have become indispensable assets in food processing, allowing for a quantitative comprehension of intricate processes and aiding

in optimization and decision-making. These models provide valuable insights into heat transfer, mass transfer, fluid flow, reaction kinetics, and microbial growth. They assist in examining various scenarios, optimizing parameters, and improving resource efficiency. While challenges like data availability and model validation persist, advancements in computational methods present opportunities for continued progress. Mathematical modelling will remain pivotal in ensuring the safety, efficiency, and sustainability of food processing practices, thereby shaping the future of the industry.

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