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Application of computational fluid dynamics simulation in predicting food protein denaturation: numerical studies on selected food products - a review*

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Highlights

- The use of CFD simulation can predict protein denaturation in food products.
- Numerical studies were conducted on selected food products to analyze protein denaturation.
- CFD simulation provides a powerful tool for optimizing food processing technologies.
- The results from the numerical studies can be used to improve the quality and safety of food products.
- The application of CFD simulation can lead to more efficient and sustainable food production practices.

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Protein denaturation is a common process in the food industry, which can impact food quality and safety. Computational Fluid Dynamics (CFD) is a powerful tool that can be used to predict protein denaturation in food products. In this review article, we present an overview of the application of CFD simulation in predicting protein denaturation in food products. We discuss the factors that influence protein denaturation, the importance of predicting protein denaturation, and the various numerical methods used in protein denaturation studies. The main focus of the article is the use of CFD simulation in predicting protein denaturation in selected food products, such as milk, meat, and eggs. We provide examples of numerical studies that have been conducted on these products, and we discuss the results and implications of these studies. The use of CFD simulation can help to optimize food processing conditions, improve food quality and safety, and reduce waste and costs in the food industry. Overall, this review article highlights the importance of using advanced computational tools such as CFD simulation in food science, research and development.

KEY WORDS: Computational Fluid Dynamics / Protein Denaturation / Food Processing / Numerical Studies / Predictive Modeling

Practical Application

The use of Computational Fluid Dynamics (CFD) simulations in predicting protein denaturation in food has great practical applications in the food industry. By using CFD simulations, food manufacturers can optimize their production processes to improve product quality, safety, and consistency. One practical application of CFD simulations is in the development of new food products. With CFD, food scientists can simulate how different processing conditions affect protein denaturation in food products. This knowledge can be used to design new products with desirable texture, taste, and nutritional qualities. Another application of CFD is in quality control. By simulating the thermal and mechanical stresses that food products undergo during processing, manufacturers can identify potential quality issues before the products hit the market. This can help reduce waste, improve customer's satisfaction, and ultimately increase profitability. CFD simulations can also be used to optimize processing conditions for existing products. By simulating the behaviour of food products under different processing conditions, manufacturers can identify the optimal conditions for achieving the desired product. This can help reduce production costs, improve product consistency, and increase production capacity. Overall, the practical applications of CFD simulations in predicting protein denaturation in food are vast and varied. By using this technology, food processors can improve product quality, safety, and consistency, reduce production costs, and ultimately increase profitability. As CFD technology continues to evolve and improve, it is likely that its applications in the food industry will continue to expand, providing even greater benefits to food manufacturers and consumers alike.

Abbreviations

Abbreviation	Full name
CFD	– Computational Fluid Dynamics
CD	– Circular Dichroism Spectroscopy
DLS	– Dynamic Light Scattering
DSC	– Differential Scanning Calorimetry
ELISA	– Enzyme-Linked Immunosorbent Assay
EY	– Egg yolk
HMF model	– 5-hydroxymethylfurfural Model
HPLC	– High-Performance Liquid Chromatography
ITC	– Isothermal Titration Calorimetry
MD simulation	– Molecular Dynamics simulation
MS	– Mass Spectrometry
NMR	– Nuclear Magnetic Resonance Spectroscopy
SDS-PAGE	– Sodium Dodecyl Sulfate - PolyAcrylamide Gel Electrophoresis
SEC	– Size-Exclusion Chromatography
SSM	– Sheep Skim Milk
TDF model	– Temperature-Dependent Function model
UV-Vis	– Ultraviolet-Visible Spectrophotometry

Introduction

Protein denaturation is a common process in the food industry, which can impact food quality and safety. Denaturation refers to the process by which a protein loses its native conformation, resulting in a loss of function. This can occur due to various factors, such as changes in temperature, pH, or the presence of certain chemicals [Cai *et al.* 2020]. For example, denaturation of proteins in milk can result in the formation of curd and whey, which can affect the taste and texture of cheese [Genene *et al.* 2018; Ravash *et al.* 2022]. The denaturation of proteins in meat can sometimes result in toughening or hardening of the meat, potentially reducing its quality and value, particularly if the process is not optimized, despite the potential advantages it may offer [Ayub and Ahmad 2019, Bircan and Barringer 2002] in LTLT cooking the temperature is often close to 60°C or even 55°C. It is applicable to a wide variety of food items. Changes in physical and chemical properties (moisture, pH, nutrients, proteins, colour and flavour etc.

To address these issues, researchers and food industry professionals have turned to computational tools such as Computational Fluid Dynamics (CFD) to predict protein denaturation in food products. CFD simulation involves using numerical methods to model and analyze fluid flow, heat transfer, and other physical phenomena [Pan *et al.* 2019, Gu *et al.* 2019]. By simulating the conditions that proteins are exposed to during food processing and storage, CFD can help predict the likelihood and extent of protein denaturation.

In this article, we present an overview of the application of CFD simulation in predicting protein denaturation in food products. We discuss the factors that influence protein denaturation, the importance of predicting protein denaturation, and the various numerical methods used in protein denaturation studies. The main focus of the article is on the use of CFD simulation in predicting protein denaturation in selected food products, such as milk, meat, and eggs. We provide examples of numerical studies that have been conducted on these products, and we discuss the results and implications of these studies. Overall, this review highlights the importance of using advanced computational tools such as CFD simulation in food science research and development.

Objectives and meaning of work

The main objectives of this article are to review the current state-of-the-art in the use of Computational Fluid Dynamics (CFD) simulation to predict protein denaturation in food products, and to present numerical studies on selected food products. The article aims to highlight the importance of using advanced computational tools such as CFD simulation to better understand protein denaturation in food, and to develop effective strategies to prevent or mitigate its effects. One of the key objectives of the article is to provide a comprehensive overview of the factors that influence protein denaturation in food products, and to explain how CFD simulation can be used to predict the likelihood and extent of protein denaturation under different conditions. By presenting numerical studies on selected food products, the article aims to demonstrate the potential of CFD simulation to provide valuable insights into protein denaturation in specific food products. Another objective of the article is to highlight the importance of predicting protein denaturation in food products from both a quality and safety perspective. By understanding the factors that contribute to protein denaturation, and by developing effective strategies to prevent or mitigate its effects, it is possible to improve the quality and safety of food products. Overall, the significance of this article lies in its contribution to the field of food science and technology, by providing a comprehensive overview of the application of CFD simulation in predicting protein denaturation in food products. The article's insights and findings can be used by researchers, food industry professionals, and policymakers to develop more effective strategies to prevent or mitigate the negative effects of protein denaturation in food products.

Factors influencing protein denaturation

Protein denaturation is a process in which proteins lose their tertiary and/or quaternary structure, leading to the loss of their biological function. Factors influencing protein denaturation include:

- Temperature - high temperatures accelerate the movements of molecules, which can lead to damage of chemical bonds in the protein structure. High

temperature is a factor that leads to protein denaturation. At increased temperatures, protein molecules gain more kinetic energy, resulting in movements in their structure that can lead to degradation of their structure [Gregersen *et al*. 2019, van Lieshout *et al*. 2020].

- pH - changes in pH can affect the electric charge of proteins, which can impact their structure and function. Change in pH is one of the factors that leads to protein denaturation. Most proteins have an optimal pH at which they maintain their structure and functionality. Changes in pH beyond this optimal range can result in changes in the electric charge of protein amino acids, which affects their spatial structure [Khan *et al*. 2019, Kamal *et al*. 2021].
- Organic solvents - proteins are typically soluble in water, but organic solvents (such as alcohol) can impact the protein structure by altering the interactions between amino acids [Bose *et al.* 2021, Kim *et al.* 2021].
- Detergents - detergents, such as SDS, can affect the protein structure through denaturation and dissolution of its structure. The presence of detergents, salts, or organic denaturants can also lead to protein denaturation, as these factors affect the electrostatic and hydrophobic stability inside the protein [Li *et al.* 2022a, Lohi *et al*. 2021].
- UV radiation - UV radiation can lead to damage of chemical bonds in the protein structure [Liu *et al.* 2019].
- Pressure - high pressure can affect the protein structure, especially in the case of proteins from organisms living in the depths of the ocean, where very high pressures prevail. High pressure processing (HPP) can cause some protein denaturation, which involves the unfolding or alteration of protein structures. This can be reversible or irreversible, depending on the intensity and duration of the pressure applied. In some cases, denaturation can lead to changes in the texture and appearance of food products [Velazquez *et al*. 2021].
- Ionizing radiation - high doses of ionizing radiation (e.g. X-ray radiation) can damage the protein structure by ejecting electrons from atoms and/or changing the electric charges on the surface of the protein [Kim *et al.* 2020].

All of these factors can impact protein denaturation by causing changes in the interactions between amino acids, resulting in changes in the tertiary or quaternary structure of the protein.

Hazards associated with protein denaturation in food products

Protein denaturation in food products can have a number of negative consequences, including changes in the texture, taste, and nutritional value of the food, as well as potential safety hazards. Here, we will discuss some of the main risks associated with protein denaturation in food products.

First and foremost, denatured proteins can affect the nutritional value of food products. Proteins are an important source of amino acids, which are essential building

blocks for the body. However, denaturation can lead to a loss of nutritional value by altering the structure and function of proteins. For example, denatured proteins in milk can lead to a loss of essential amino acids, reducing the nutritional quality of the milk [Abbring et al. 2020, Horstman and Huppertz 2022].

In addition to affecting the nutritional value of food products, denatured proteins can also pose safety risks. For example, denatured proteins in meat can provide a substrate for the growth of bacteria, increasing the risk of foodborne illness. Denatured proteins can also affect the texture and appearance of food products, making them less appealing to consumers [Kovaleva *et al.* 2021].

Another risk associated with protein denaturation in food products is the potential for allergenicity. Denatured proteins can have different structural and functional properties than native proteins, and this can lead to an increase in allergenicity. For example, denatured proteins in peanuts have been shown to be more allergenic than native proteins [Ahmed *et al.* 2021, Geng *et al.* 2023].

Overall, protein denaturation in food products can have a number of negative consequences. As such, it is important to understand the factors that contribute to denaturation and to develop effective strategies to prevent or mitigate its effects. Computational tools such as CFD simulation can be a valuable tool in predicting protein denaturation in food products, allowing for more effective strategies to be developed to ensure food safety and quality.

Numerical methods in protein denaturation studies

The use of computational methods has become increasingly important in the field of food science and technology, including in the study of protein denaturation. In this chapter, we will discuss some of the main numerical methods used in the study of protein denaturation, including both CFD simulation and molecular dynamics (MD) simulation [Hollingsworth and Dror 2018].

CFD simulation is a widely used numerical method for predicting the flow of fluids and gases in complex systems [Ghafori 2020, Li *et al*. 2022, Masud *et al.* 2019, Promtong *et al*. 2020]. In the context of protein denaturation, CFD simulation can be used to predict the local temperature, pressure, and shear stress in food products, which are important factors that influence protein denaturation [Salish *et al*. 2021, Wazed and Farid 2019, Dreckmann *et al*. 2020, McHardy *et al.* 2021]. CFD simulation can also be used to predict the mass transfer of water, solutes, and gases in food products, which can affect the kinetics of protein denaturation. By combining CFD simulation with experimental data, it is possible to develop more accurate and realistic models of protein denaturation in food products [Azmir *et al*. 2019, Albuquerque *et al.* 2019, Prabhakar *et al*. 2021].

MD simulation is another numerical method that has been used to study protein denaturation. MD simulation involves the use of computer algorithms to simulate the movement and interaction of atoms and molecules over time. In the context of protein

denaturation, MD simulation can be used to predict the structural changes that occur in proteins under different conditions, such as changes in temperature or pH. By simulating the folding and unfolding of proteins at the atomic level, MD simulation can provide insights into the mechanisms of protein denaturation, and can be used to develop new strategies to prevent or mitigate its effects [Hollingsworth and Dror 2018].

In conclusion, the use of numerical methods such as CFD simulation and MD simulation can provide valuable insights into the mechanisms of protein denaturation in food products. By combining numerical simulations with experimental data, it is possible to develop more accurate and realistic models of protein denaturation, and to develop more effective strategies to prevent or mitigate its effects.

CFD simulations in protein denaturation studies

In recent years, computational fluid dynamics (CFD) simulation has emerged as a powerful tool for predicting protein denaturation in food products. CFD simulation involves the use of computer algorithms to simulate the flow of fluids and gases in complex systems, and can be used to predict local temperature, pressure, and shear stress in food products, which are key factors that influence protein denaturation.

One of the main advantages of CFD simulation is that it allows for the analysis of fluid flow and heat transfer in three dimensions, which can provide a more accurate and detailed understanding of the dynamics of protein denaturation in food products. CFD simulation can be used to predict the transport of heat and mass in food products, which are important factors that affect the kinetics of protein denaturation. CFD simulation can also be used to predict the impact of different processing conditions on protein denaturation in food products. For example, CFD simulation can be used to study the effects of different cooking temperatures and times on protein denaturation in meat products. By predicting the temperature and stress distributions in meat during cooking, CFD simulation can provide valuable insights into the mechanisms of protein denaturation and help to optimize cooking conditions to minimize protein denaturation [Nethery *et al*. 2022, Muga *et al*. 2021]. Finally, CFD simulation can be used to optimize food processing and storage conditions to prevent protein denaturation. For example, CFD simulation can be used to predict the temperature and airflow patterns in food storage facilities, which can help to minimize the risk of protein denaturation due to temperature fluctuations [Chauhan *et al*. 2019, Tasiya and Gajdhar 2021, Yildiz 2019, Söylemez *et al*. 2021].

In conclusion, CFD simulation is a powerful tool for predicting protein denaturation in food products. By providing a detailed understanding of the dynamics of protein denaturation under different conditions, CFD simulation can help to optimize food processing and storage conditions to prevent protein denaturation and maintain the quality and safety of food products.

Mathematical models describing protein denaturation processes

In addition to the use of computational fluid dynamics (CFD) simulation, mathematical models can also be used to describe the process of protein denaturation in food products. These models can be used to predict the kinetics of protein denaturation under different processing conditions and to identify the factors that contribute to protein denaturation.

One of the most widely used mathematical models for predicting protein denaturation in food products is the Arrhenius equation, which describes the temperature dependence of the rate of protein denaturation. The Arrhenius equation states that the rate of protein denaturation increases exponentially with increasing temperature, and can be used to predict the rate of denaturation at different temperatures.

In addition to the Arrhenius equation, there are also other mathematical models used to describe protein denaturation processes in food products. Some of them are listed below:

- Kinetic model based on the quadratic equation of mass action: describes the kinetics of protein denaturation depending on protein concentration, temperature, and pH [Chellaboina *et al.* 2009].
- HMF model: describes protein denaturation in the presence of 5-hydroxymethylfurfural (HMF), a substance that forms as a result of reducing reaction between sugar and amino acids [Kowalski *et al.* 2013].
- Reversible denaturation model: describes denaturation and renaturation processes as reversible processes that can be described using thermodynamic equations [Brandts and Brandts 1964].
- Temperature-Dependent Function (TDF) model: describes protein denaturation as a function of temperature and time [Otsuka *et al*. 2021].
- Power-law cutting model: describes structural changes in proteins depending on time and temperature, using the concept of cutting power, which is the amount of energy needed to remove a certain amount of protein from the solution [Sawada and Honda 2006].

Each of these models has its strengths and limitations and can be used depending on the specifics of the food products being studied and processing conditions. Other mathematical models that have been used to describe protein denaturation in food products include the Weibull model, which describes the probability of protein denaturation as a function of time and temperature [Santillana Farakos *et al*. 2013, Boekel 2008], and the reaction rate model, which describes the kinetics of protein denaturation as a function of temperature, pH, and other factors [Bischof and He 2005]. Mathematical models can also be used to predict the effect of processing conditions on protein denaturation in food products. For example, models can be used to predict the impact of different cooking temperatures and times on the kinetics of protein denaturation in meat products.

While mathematical models can provide valuable insights into the process of protein denaturation, they are often limited by the complexity of the underlying

processes and the availability of data to support the models. CFD simulation can provide a more detailed and accurate understanding of the dynamics of protein denaturation in food products and can be used to complement mathematical models to optimize food processing and storage conditions.

Tools for thermodynamic and kinetic analysis of processes occurring in investigated food products

Thermodynamic and kinetic analysis of the denaturation processes in food products is essential for understanding the underlying mechanisms and predicting the stability of protein-based food products. In this chapter, we will discuss the tools and methods used for such analyses. Thermodynamic analysis involves the determination of thermodynamic parameters, such as enthalpy, entropy, and Gibbs free energy, which describe the stability of proteins in various conditions [Stewart *et al.*, 2023; Li *et al.*, 2021] most experiments are conducted in dilute buffered solutions. To resolve the effect of crowding on protein stability, we use 19F nuclear magnetic resonance spectroscopy to follow the reversible, two-state unfolding thermodynamics of the N-terminal Src homology 3 domain of the Drosophila signal transduction protein drk in the presence of polyethylene glycols (PEGs). The most commonly used method for thermodynamic analysis is differential scanning calorimetry (DSC), which measures the heat absorbed or released by proteins as they undergo temperature-induced denaturation [Agafonkina *et al.* 2019]. Kinetic analysis involves the determination of reaction rates and rate constants, which describe the speed of the denaturation process. The most commonly used method for kinetic analysis is UV-Vis spectrophotometry, which measures the absorbance of light by the protein as it denatures [Zhang *et al.* 2021]. Other tools that can be used for thermodynamic and kinetic analysis include isothermal titration calorimetry (ITC), dynamic light scattering (DLS), and circular dichroism (CD) spectroscopy [Santa Rosa *et al.* 2021, Andlinger *et al.* 2022, Akita *et al.* 2020]. These tools and methods allow for a more comprehensive analysis of the denaturation processes in food products, which can aid in the development of more stable and higher quality protein-based food products.

Below are listed some of the tools commonly used for the thermodynamic and kinetic analysis of processes occurring in food products, among others:

- Differential scanning calorimetry (DSC).
- UV-Vis spectrophotometry.
- Isothermal titration calorimetry (ITC).
- Dynamic light scattering (DLS).
- Circular dichroism (CD) spectroscopy.
- Fluorescence spectroscopy [Farrokhi *et al*. 2019; Singh and Amamcharla 2021].
- Fourier transform infrared (FTIR) spectroscopy [Sun *et al.* 2022a, Li *et al.* 2023].

- Nuclear magnetic resonance (NMR) spectroscopy [Wang *et al*. 2020, Cai *et al.* 2019].
- X-ray crystallography.
- Mass spectrometry [Stachniuk *et al*. 2021, Buecker *et al*. 2022].
- High-performance liquid chromatography (HPLC) [Häfner *et al*. 2021, Sadeghi *et al*. 2023].
- Size-exclusion chromatography (SEC) [Chung *et al.* 2022, Hannß *et al*. 2020]
- Gel electrophoresis (SDS-PAGE, native-PAGE) [Hashim *et al*., 2019, Sharma *et al.* 2021].
- Enzyme-linked immunosorbent assay (ELISA) [Koppelman *et al*. 2021, Yamasaki *et al*. 2022].

The application of CFD simulations in predicting protein denaturation in food

Numerical studies on protein denaturation in milk

In the process of pasteurizing milk and its derivatives using plate heat exchangers, protein fouling poses a limitation due to the denaturation and aggregation of β-lactoglobulin (BLG) on the heat transfer surface. This study focuses on modeling the heat-induced denaturation mechanisms of BLG using a 2D computational fluid dynamics (CFD) analysis. The validity of the numerical model is demonstrated through intermediate validations that confirm its ability to capture the hydrodynamics and produce results consistent with experimental data. The close agreement between the denaturation levels obtained from the CFD model and experimental measurements indicates the model's capability to simulate the chemical reaction. The analysis of species distribution in the plate heat exchanger, based on CFD data, reveals that unfolded BLG species (N - native β-lg, U - unfolded β-lg and A - aggregated β-lg) act as precursors for deposits, and their distribution correlates with deposit formation. The study highlights the importance of considering temperature and velocity heterogeneities in plate heat exchangers. This research contributes to validating the chemical kinetic model used to describe protein deposits and paves the way for developing models to prevent deposits and optimize milk heat treatment processes [Bouvier *et al.* 2014].

Another study focused on simulating protein denaturation during the spray drying of camel milk using Computational Fluid Dynamics (CFD). The goal was to identify suitable quality indicators for CFD simulation. The spray drying experiment varied the drying temperature from 140-200°C while keeping other parameters constant. The moisture content and yield of camel milk powder were influenced by temperature, with an inverse relationship observed above 160°C. CFD successfully predicted outlet temperatures with satisfactory agreement to experimental measurements. The solubility of specific milk proteins correlated well with the CFD-predicted temperature profiles. For camel milk, caseins and Bovine Serum Albumin (BSA)

showed good variations with temperature, making them suitable indicators for loss of solubility during spray drying. Scanning Electron Microscopy (SEM) revealed that higher temperatures produced round-type powders. These findings contribute to the understanding of protein denaturation and quality indicators in spray drying processes for camel milk [Habtegebriel *et al.* 2021].

A new model combining whey protein thermal inactivation and Computational Fluid Dynamics (CFD) has been developed for skim milk spray drying. The model incorporates evaporation and particle formation models to calculate particle moisture contents, temperatures, and residence times. A quality model based on Williams-Landel-Ferry equations for inactivation kinetics was implemented into the CFD code and validated against experimental data from skim milk spray drying. The comparison of protein activity levels obtained from the CFD simulations with data from differential scanning calorimetry (DSC) showed good agreement. The simulations demonstrated that higher feed rates result in lower loss of whey protein activity due to lower temperature fields. The implementation of the whey protein inactivation model within the CFD solver provides a means to determine protein concentration in spray-dried powders, enhancing the understanding and control of the spray drying process [Jaskulski *et al.* 2017].

In the study by Liu *et al*. [2020], the thermal denaturation of lactoferrin in unprocessed bovine milk was investigated across a range of temperatures from 65 to 121°C, with varying holding times. Two sources of milk (New Zealand and China), were used, each with varying levels of naturally occurring iron saturation in lactoferrin. It was observed that lactoferrin in the Chinese milk exhibited higher denaturation rates compared to the New Zealand milk at temperatures up to 80°C. However, at 85°C, denaturation rates in both types of milk were similar but significantly higher than at 65°C. At 95°C, lactoferrin in the New Zealand milk denatured at a faster rate than in the Chinese milk. Based on these findings, a combined kinetic and Arrhenius-based model was developed and validated to estimate the retention of native lactoferrin under different temperature-time conditions. This model can be useful for evaluating and improving lactoferrin retention during food manufacturing processes.

Liu *et al*. [2022] investigated the influence of calcium on whey protein fouling behavior in plate heat exchangers (PHEs) using a benchtop fouling device designed to mimic PHE conditions in a laminar regime. Computational fluid dynamics was employed to simulate the thermal denaturation and deposition of β-lactoglobulin (BLG) in the microchannel. The model was validated by experimental measurements of the bulk fluid temperature using fluorescence microscopy. Results demonstrated a linear relationship between the pre-exponential factor of the deposition reaction and calcium concentration, indicating that fouling occurs with one calcium ion per BLG molecule. In-situ imaging of fouling deposits revealed spherical structures at low calcium levels and denser, rod-like structures at higher concentrations. The fouling behavior displayed a crystallization-like pattern, with a preference for previously fouled layers over clean surfaces. These findings confirm the crucial role of ionic calcium in fouling

deposit formation, facilitating the anchoring of denatured BLG and protein-protein interactions. The benchtop fouling device offers a simplified approach for studying fouling phenomena with real-time optical measurements, providing valuable insights for energy and material-efficient processes compared to traditional PHEs.

In another study the interactions among proteins in sheep skim milk were investigated during heat treatments at temperatures ranging from 67.5 to 90°C for durations of 0.5 to 30 minutes. The denaturation kinetics of whey proteins, association of denatured whey proteins with casein micelles, and changes in the size and structure of casein micelles were characterized. The level of denaturation and association with casein micelles increased with higher temperatures and longer heating times, with β-lactoglobulin (β-LG) exhibiting faster rates compared to α-lactalbumin (α-LA) in the temperature range of 80 to 90°C. The casein micelle size increased depending on the heating conditions, with a significant increase observed after reaching a 95% association level with denatured whey proteins. The size increase was attributed to both whey protein association and casein micelle aggregation. These findings highlight the importance of understanding protein denaturation and micelle changes during heat treatments in SSM. Further research is warranted to explore the formation of larger aggregates and their impact on the heat stability of sheep milk [Pan *et al*. 2021].

Van Boekel [2022] discussed advancements in protein denaturation modeling, focusing on kinetic analysis. It explores the use of computational tools such as Bayesian regression, nonlinear regression, and multiresponse analysis in studying heat-induced chemical changes and protein denaturation in dairy products. The importance of predictive power and proper statistical analysis is emphasized. The application of these modeling techniques can aid in product design, quality optimization, and shelf life prediction. Researchers are encouraged to propose, analyze, and test kinetic models while considering scientific underpinnings, clear assumptions, parameter uncertainties, and predictive capacity. Bayesian approaches offer advantages in model interpretation and parameter understanding. This overview provides valuable insights for researchers generating kinetic data and enables critical evaluation of published models for protein denaturation, however Warncke *et al*. [2022] study aimed to understand the mechanisms behind changes in viscosity when increasing the total protein concentration, altering the casein/whey protein ratio, and applying heat treatment in fresh/hard cheese and quark production. The viscosity of unheated and heated milk protein concentrates with varying total protein concentrations (3-14%) and casein/whey protein ratios (85:15, 92:8, 98:2) was analyzed. The results revealed that a 37% depletion of whey protein was sufficient to counteract the impact of repulsive forces from casein micelles on viscosity, achieve the highest particle packing density and polydispersity in the concentrates, and allow for up to 95% denaturation of whey proteins without affecting the viscosity after heating. These findings provide insights into optimizing protein concentration and denaturation for specific dairy product processing.

Numerical studies on protein denaturation in meat

Chapwanya and Misra [2015] study focused on the mathematical modeling of protein denaturation, specifically in the context of double-sided heat-treatment of meat. A mathematical model for simultaneous heat and mass transfer was developed using constitutive equations based on Fourier conduction and the Flory-Huggins theory. The model was verified through a reduced one-dimensional case and showed good agreement with experimental findings. The model successfully predicts the core temperature of the beefsteak, although it has some limitations for thicker steaks. Sensitivity analysis highlights the importance of selecting the initial porosity of the meat for accurate predictions. The model can be extended to other cooking methods, such as single-sided heating with flipping, roasting, or frying, by modifying the boundary conditions. Incorporating equations for microbial inactivation would enable predictions of microbial safety. This model contributes to the understanding of protein denaturation in food processing and can be valuable for optimizing cooking processes and ensuring food safety.

Feng *et al*. [2021] investigated the impact of oxidative treatment on sarcoplasmic proteins (SPs) and its influence on the properties of pork myofibrillar proteins (MPs) gel. Oxidation of SPs led to increased carbonyl content, decreased total sulfhydryl content, and the formation of cross-linkages through disulfide and covalent bonds. The addition of oxidized SPs to MPs gel resulted in enhanced gel strength but reduced water holding capacity (WHC). The microstructure of the composite gel with moderately oxidized SPs showed a more compact network with smaller pores, indicating the expulsion of trapped water. Further analysis revealed increased environmental polarity of aliphatic C-H groups with SPs oxidation. This study contributed to understanding the relationship between SPs oxidation and MPs gel properties in meat processing, enabling better quality control of gel-based meat products. Future research can explore the interaction mechanism between SPs and MPs co-oxidation and its impact on gel properties.

He *et al.* [2019] paper focused on the modeling of protein denaturation in false abalone during wet heating at 95-100°C. A heat transfer model was developed to predict the degree of myosin and actin denaturation. The effects of cooking time on water mobility, tenderness, and sensory acceptability were assessed. The results from 3D finite element heat transfer analysis and reaction kinetics showed that muscle proteins were completely denatured within 60-80 seconds of wet heating. Analysis using low field 1H nuclear magnetic resonance (LF-NMR) and magnetic resonance imaging (MRI) revealed a reduction in immobilized water content and decreased shear force with extended cooking time. Sensory acceptability decreased with longer cooking times. Partial least squares (PLS) analysis demonstrated a strong correlation between immobilized water, color, taste, and sensory acceptability. These findings contribute to a better understanding of quality assessment and control in seafood cooking. Further research is needed to explore the relationships between cooking parameters and microstructural changes during prolonged cooking.

In Nelson *et al.* [2020] study, a precise two-dimensional mathematical model for protein denaturation during steak cooking was proposed, employing the Flory-Rehner theory. The model considers meat as a poroelastic medium saturated with fluid, accounting for the effects of heat on protein matrix deformation and moisture loss, resulting in shrinkage. Numerical simulations conducted demonstrate excellent agreement with experimental data, validating the accuracy of the proposed model. Additionally, a novel and computationally efficient approach to incorporate shrinkage in the model is introduced. This research contributed to a deeper understanding of protein denaturation during steak cooking and provides a valuable tool for predicting cooking outcomes.

Mathematical modeling plays a crucial role in understanding protein denaturation, a process of great significance in various domains. Onyeaka *et al*. [2022] review focused on the application of mathematical models to elucidate protein denaturation, with a particular emphasis on sous vide cooking. Sous vide cooking, characterized by low-temperature cooking of vacuum-sealed foods, offers numerous benefits in terms of product quality and sensory attributes [Wojtasik-Kalinowska *et al*. 2021]. However, the lower temperatures used in sous vide raise concerns regarding microbiological safety and protein denaturation. Mathematical modeling has been employed to optimize sous vide processing parameters, aiming to maximize quality characteristics while minimizing the risk from food pathogens. These models aid in predicting protein stability and designing strategies to mitigate denaturation-induced loss of function. Future applications of mathematical modeling in sous vide processing should focus on optimizing process conditions and cooking methods for different types of foods and sizes of products. Furthermore, a more comprehensive modeling approach, real-time quality evaluation, and the implementation of hurdle technology are promising areas for further investigation. In conclusion, mathematical modeling provides valuable insights into protein denaturation during sous vide cooking, enabling the optimization of processing parameters to enhance food quality and ensure microbiological safety. The continued advancement of mathematical models will contribute to the ongoing improvement of sous vide cooking techniques and their application in various food preparations.

In van der Sman [2017] paper, a model was proposed to predict the electrical conductivity of muscle meat, specifically for evaluating Ohmic heating. The model considers the composition, temperature, and microstructure of the meat, including protein, water, salt, muscle fiber orientation, and the development of drip channels caused by protein denaturation. It also incorporates protein denaturation kinetics. The model has been validated for various types of meat with different compositions and heating rates, using DSC measurements to validate the submodel for protein denaturation. Results indicate that for meats heated rapidly, the conductivity increases linearly with temperature, as protein denaturation and drip channel formation are absent. However, for slower heating rates, the conductivity exhibits nonlinear behavior, with a significant decrease at temperatures above 70°C, attributed to complete protein

denaturation. The study highlights the potential of Ohmic heating at fast rates to retain moisture in meat during the heating process.

Another study conducted by Szpicer *et al*. [2022] focused specifically on the denaturation of proteins in beef during heat treatment. The authors utilized CFD simulations to model the denaturation degree of beef proteins under various processing conditions, such as temperature and time. The results of the study showed that CFD simulations can be a valuable tool in optimizing the heat treatment of beef to achieve desired levels of denaturation and quality. This demonstrates the potential of numerical studies in the food industry to not only understand protein denaturation but also to optimize food processing for improved product quality [Szpicer *et al*. 2022].

Numerical studies on protein denaturation in eggs

Protein denaturation is a complex process that plays a crucial role in various biological and industrial applications. Understanding and modeling the denaturation process is essential for optimizing protein functionality and stability. Capuano and Janssen [2021] review focused on the modeling of protein denaturation, discussing the various approaches and techniques used to study and simulate the structural changes that occur during denaturation. Different computational methods, such as molecular dynamics simulations, Monte Carlo simulations, and coarse-grained models, are explored for their ability to capture the thermodynamic and kinetic aspects of denaturation. Additionally, experimental techniques, such as spectroscopy and calorimetry, are combined with computational models to validate and refine the denaturation models. The challenges and limitations of current modeling approaches are also discussed, highlighting the need for further development of accurate and comprehensive models to predict protein denaturation behavior under different conditions. Improved modeling of protein denaturation will provide valuable insights into protein folding, stability, and functionality, enabling the design of novel proteins for various applications in biotechnology and food science.

Pero *et al.* [2019] study focused on the modeling of protein denaturation, specifically in the context of thermal processing of egg white. A numerical model based on the finite volume method was developed to simulate the heat transfer, coagulation, and fluid flow during the heating process of liquid egg white. Experimental investigations were conducted, and the temperature profile and coagulated phase front were recorded. The model successfully predicted the temperature history and coagulated phase front, and the results were compared to those of fresh eggs, water, and coagulated egg models. The simulation accurately represented the thermal processing of egg white, providing a valuable tool for process optimization in the industry. The study also highlighted the potential application of the model in the processing of intact shell eggs to control microbial load while preventing egg white coagulation. Future research could focus on incorporating the cooling section of the thermal process for a more comprehensive analysis.

Suhag *et al.* [2022] paper focused on the modeling of protein denaturation process. The effects of microfluidization at different pressures on the rheological characteristics of liquid egg yolk (EY) were investigated. The apparent viscosity of EY increased with increasing microfluidization pressure, indicating changes in protein structure. Rheological models, including Power law, Bingham, Casson, and Herschel-Bulkley models, successfully described the experimental data. Time-dependent rheology revealed thixotropic and anti-thixotropic behavior in microfluidized EY. Dynamic rheological analysis showed a transition from solid-like to liquid-like behavior as the microfluidization pressure increased. The proposed model successfully predicted the unfolding of EY proteins during the microfluidization process. These findings contribute to the understanding of protein denaturation and have implications for food processing, particularly in the development of new products and optimization of industrial processes. The model can be utilized in designing efficient denaturation processes for various protein-rich food products.

Numerical studies on protein denaturation in cereals and cereal products

Sun et al. [2022] study utilized numerical simulation to investigate the denaturation of soybean protein isolate (SPI) during extrusion under various screw speeds and combinations. By analyzing fluid-dynamic parameters, such as shear rate distribution, shear viscosity distribution, and residence time, combined with extrudate properties, the effects of screw speed on SPI denaturation are examined. The results indicate that increasing the screw speed enhances the shear rate, reduces the shear viscosity of the SPI fluid, and decreases the residence time, leading to increased denaturation. The regions with the highest shear rate and lowest shear viscosity are observed at the screw flight flanks, where the SPI fluid undergoes alternating shearing forces. Additionally, a narrower axial channel width is found to significantly enhance the denaturation of molten proteins. Consequently, extrudates produced at relatively high screw speeds (140 rpm) exhibit a homogenous structure, smooth surface, and favorable color and texture profiles, indicating successful denaturation of the SPI proteins.

Extrusion cooking is gaining attention as a technology for producing protein-based products with improved functionality. However, the understanding of protein denaturation during extrusion is still limited. Mosibo *et al.* [2022] review aimed to provide an overview of the current knowledge and research on modeling protein denaturation during extrusion. Various studies on vegetable, animal, and insect proteins are examined to explore the potential of extrusion in improving protein functionality. The effects of processing variables such as barrel temperature profile, screw speed, and moisture content on protein denaturation are discussed. Mathematical and predictive models are essential for comprehending the underlying mechanisms and predicting the functional properties of the final products. Computer simulation techniques, including computational fluid dynamics, can be utilized to simulate the flow and rheological characteristics of protein materials during extrusion. Moreover, factors like the molecular structure, lipid and protein content, and particle size of proteins should be

considered for achieving desired extrudate properties. Future research should focus on comprehensive studies that integrate the effects of thermal and mechanical energy input with the physicochemical changes occurring during extrusion. This will enable the development of systematic models and the production of protein-based extrudates with enhanced functionalities for various food applications.

Application of CFD simulation in predicting protein denaturation as a tool for optimizing technological processes

Numerical simulations based on computational fluid dynamics (CFD) have been widely used in recent years to study protein denaturation in various food products. CFD simulations provide a powerful tool for predicting the effects of process variables, such as temperature and pressure, on protein denaturation. This can be useful for optimizing technological processes, as it allows for the identification of the optimal process conditions that result in minimal protein denaturation.

Razmi *et al.* [2021] review paper provided an overview of recent initiatives in the modeling of spray drying processes. The initiatives are categorized into three main areas: plug-flow modeling, Computational Fluid Dynamics (CFD) modeling, and modeling of powder qualities. The plug-flow model enables rapid assessments and exploration of hypothetical scenarios. However, the difficulties involved in adapting it for counter-current spray drying applications are also addressed. The CFD modeling approach is explored, along with the common dilemmas faced in this area, and recent developments in agglomeration modeling are highlighted. The review also touches on modeling techniques for predicting specific powder qualities, such as protein denaturation and crystalline-type powder characteristics. The paper emphasizes the need for experimental validation and provides guidelines for selecting appropriate models and simulations. It suggests further development in agglomeration modeling and the prediction of agglomerate structure. Additionally, it discusses the potential of continuum and molecular scale modeling for particle surface formation prediction. Overall, while spray drying has been widely used for commercial applications, there is still much to explore and understand in terms of mathematical modeling. The review serves as a valuable resource for future modeling works and advancements in the field.

In recent years, there has been a growing interest in plant-based meat alternatives. High-moisture extrusion is a vital technology for creating plant-based meats with meat-like texture and fibrous structure. However, understanding the protein interactions and phase transition during extrusion remains a challenge. Zhang *et al.*, [2022] plant-based meat substitutes have generated considerable interest for their benefits in terms of environmental sustainability and personal health. High-moisture (above 40%) article summarized protein sources suitable for high-moisture extrusion and explains the theories behind protein texturization. It also analyzes technical aspects such as extrusion conditions, screw configuration, and cooling die design. Moreover,

the formation of fibrous structures through protein aggregation and phase separation is discussed, highlighting the need for simulation and experimental work to regulate and control the extrusion process. To accurately simulate the flow and rheological properties of materials during extrusion, 3D CFD coupled with particle tracking simulation was utilised. Finally, comprehensive evaluation methods are necessary to compare plant-based meat substitutes with animal meats, considering their fibrous structures, sensory characteristics, and nutritional composition. Although high-moisture extruded plant-based meats exhibit fibrous structures, further improvements are required in terms of texture, juiciness, and flavor.

In conclusion, the use of CFD simulation in predicting protein denaturation in food products provides a valuable tool for optimizing technological processes and improving product quality. However, it is important to note that CFD simulations have limitations, and the results should be interpreted with caution. Further research is needed to better understand the limitations of CFD simulations and to develop more accurate models for predicting protein denaturation in food products.

The use of numerical simulation results in industrial practice

The results of numerical simulations of protein denaturation in food products have great potential to be used in industrial practice. By providing a detailed understanding of the complex physical and chemical processes that occur during food processing, CFD simulations can be used to optimize processing conditions and improve product quality. In this chapter, we will discuss some examples of how the results of CFD simulations can be applied in industrial practice.

Jaskulski *et al.* [2020] article discussed the development of mathematical models and CFD simulations for the milk spray-drying process. The aim is to optimize the design of drying towers, reduce production costs, and improve spray dryer efficiency. The CFD simulations were performed for a new design of a monodisperse multi-stream atomizer. Parameters such as drying efficiency, protein thermal degradation, collision frequency, and wall deposition were obtained from the simulations. The results demonstrate the impact of geometry modifications, process parameters, and nozzle settings on dryer performance and product quality. The simulations indicate that a high and narrow co-current spray dryer with axial airflow without recirculation is the optimal construction. It prevents agglomeration, wall deposition, and overheating of particles, resulting in high-quality and uniform powder production. The findings have implications for various industries, including pharmaceuticals, cosmetics, and food powders.

In Plana-Fattori *et al.* [2020] study, CFD model was developed to investigate the thermal processing of a liquid food product containing whey proteins in a heat exchanger. The model considered the coupling between fluid flow, heat transfer, and the thermal denaturation-aggregation of whey proteins. Specifically, the focus was on studying the behavior of whey proteins in a cream cheese formulation. The

model predictions revealed that the apparent viscosity of the liquid product exhibited a complex behavior, influenced by both local temperature and the degree of whey protein denaturation. The model was flexible, allowing for changes in the length of the holding section to assess their impact on the final degree of protein denaturation.

In summary, the results of CFD simulations of protein denaturation in food products have great potential to be applied in industrial practice. By providing a detailed understanding of the physical and chemical processes that occur during food processing, CFD simulations can be used to optimize processing conditions, design and optimize food processing equipment, and develop new food products.

Conclusions

Numerical studies on selected food products present the potential of Computational Fluid Dynamics (CFD) simulations in predicting protein denaturation in various food products. The studies showed that CFD simulations can accurately predict the protein denaturation degree and spatial distribution in food products such as beef, eggs, and milk. The simulation results can be used to optimize food processing parameters and improve product quality. Furthermore, this study underscores the significance of precise protein denaturation modelling, emphasizing the necessity for experimental validation of simulation results. Combining CFD simulations with empirical data contributes to a more comprehensive understanding of the protein denaturation process within food products.

Conflicts of interest

The authors declare no conflict of interest.

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