

Modelling and Simulation in Food Packaging

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Abstract

Packaging plays a vital and indispensable role in the food processing industry. It not only helps extend the shelf life of food products but also serves as a powerful tool for marketing and consumer engagement. Designing an effective food package is a complex task that requires careful consideration of multiple factors influencing the product during storage, transportation, and handling. The design must also meet consumer expectations while ensuring the desired shelf-life extension. In recent years, modeling and simulation techniques have emerged as advanced, reliable, and efficient tools for food package design. These methods surpass traditional trial-and-error approaches by providing data-driven insights. Various modeling techniques—such as deterministic chemical safety modeling, physics-based modeling, and life cycle assessment (LCA) modeling are used to optimize package performance and sustainability. The deterministic chemical safety model focuses on the physicochemical interactions between food and packaging materials, including migration behaviour, temperature effects, and water activity. Physics-based models employ Finite Element Analysis (FEA) and Computational Fluid Dynamics (CFD) to evaluate mechanical forces, structural stability, heat transfer, and fluid flow. Meanwhile, LCA modeling assesses the environmental impact of packaging systems, supporting the development of sustainable materials and processes. Although these techniques are faster, more reliable, and cost-effective than conventional methods, they require skilled expertise, accurate data, and careful setup for optimal performance.

Key words: Packaging, modeling, simulation, computational fluid dynamics, finite elemental analysis, life assessment cycle

1. Introduction

Food is the fundamental need of life, and it comprises multiple interconnected processes such as food production, processing, marketing and distribution. These processes are helpful in enhancing the shelf life of food products, but the food wastage is still a major concern for food industries, environment, economic and social implications. The problem is mainly associated with perishability of foods which because of biochemical deterioration and microbial contamination make unsafe for consumption and storage (Yang et al., 2025). Hence, there is a need for techniques to enhance the shelf life of foods (Swetha B. S. et al., 2024). With all innovative processing and storage techniques, Packaging also plays a major role for enhancing the shelf life of food products. Packaging acts as a mirror for food product. It is a reflection of products characteristics. Also, package characteristics such as design, convenience to handle and use, communication, hygiene, recyclability highly influences the buying ability of the consumers. The right selection of packaging material, consumer oriented, innovative as well as personalized designs of packages helps in improving the shelf life of food, can reduce the problem of the food wastage (Yuehui Ye, Ziming Ye, Lushan Guo, 2025).

Packaging is an important integral part of the food industry. Packaging serves four major functions: convenience, containment, communication and protection. Packaging provides barrier against physical, chemical, and biological factors. It is responsible for maintaining the quality of food products during storage, preventing the loss of volatile components and protecting the food products from external agents like microorganisms, gases, water vapour, light etc. (Marangoni Júnior et al., 2022). The selection of packaging materials depends on the desired physical and technical characteristics of the final packaging material as well as the type of food product needs to be packed. Globally, four major types of materials, glass, metal, paper and paperboard and plastics are used for manufacturing of rigid (can, jars, bottles, caps), semi-rigid (boxes, caps, closures) and flexible packages (wraps, wraps, tubes). The packaging either can be used as a mono-packaging or as multi-packaging such as laminates, composites etc. to improve the properties of packaging materials (Lacourt et al., 2024). For example, metals and glasses provide effective barrier against chemical factors (moisture and gases) but need closures (usually made of plastics) to assist filling and emptying. Plastics provide

good strength, but they have little permeability for gases, hence needed gasket material for sealing of the caps. Paper based packaging materials such as paperboard and corrugates boxes act as good physical barriers and resist impacts, adhesions and crushing damage. Papers and shredded plastics are also used cushioning materials to protect the foods from impact mechanical damages, skin wearing and tearing (Marsh & Bugusu, 2007). Research has showed that global consumption of glass, metal and paper-based packaging materials is around 11%, 6% and 34% respectively. Plastic based packaging materials serve good physical and chemical properties. They are light weight, resilient, modular, less expensive and can be reused and recycled easily. These characteristics make plastics more desirable than other packaging materials and around 37% of packaging materials is manufactured using plastics (Lacourt et al., 2024).

Despite all these advantages, food packaging can have some negative environmental impact. The petrochemical origin of plastics, need of high energy and recycling, short usage span, emission of harmful chemicals during food contact and difficulty in biodegradation. Also, a traditional packaging material alone are difficult in providing all physical, chemical and biological barrier properties. They are also less effective in real time communication against spoilage, adulteration and change in product's environment. All these factors have created a need to design a safe, smart and sustainable alternative of traditional packaging materials (Lacourt et al., 2024) and there is a need for adaptation of circular economy. For achieving these goals, design of a food packaging material needs to focus on: development and improvement in packaging process, reducing the environmental impact of packaging, and implications of regulatory compliance for packaging materials (Marangoni Júnior et al., 2022).

Packaging design is an innovative process. It includes various steps of conceptualizing, planning, modelling and simulation, and development of a package or a container. The structure of the package, selection of materials, functionality and visual appearance depends on the consumer's requirements (Srivastava et al., 2022). A well-designed package creates a balance between environmental, economic and social considerations. It protects the food from physical, chemical and biological factors and helps in reducing the food loss. Compact, convenient and innovative designs attract consumer and increase the product demand by communicating about quality and history of product. For example, a package developed using biomaterials like Poly Lactic Acid (PLA), polysaccharides, chitosan etc. will help in achieving sustainability. Use of different colours, materials and shapes helps to create brand value (Pavón Losada et al., 2025). Traditionally, the packaging materials are designed using traditional empirical approaches. These approaches are considerably relied on resources-intensive iterative prototyping and physical stress testing methods. These methods are expensive, time consuming and generate a lot of waste. Therefore, these approaches are increasingly replaced by computational modeling and simulation techniques.

2. Literature Review

Modeling and simulation are an important and essential part of designing. Modeling is a process of developing a simplified image of a real-world system using computer programs. The developed models help to study the system easily and conveniently. Simulation is the process of observing and analyzing a system's behaviour by running a model over time. It uses different mathematical equations and computer programs to solve the system numerically. Both modeling and simulation are the advanced designing tools which are commonly used to study the packaging system's performance under different conditions such as stress, drop impact, environment change, migration of water vapours and gases etc. They help researchers to optimize the packaging structuring and manufacturing conditions, material selection, prediction of the package shelf life, improves the process efficiency and ensure the safety and quality of the package under tested conditions (Menner, 1955). They help the industries to minimize the proto-typing and testing cost, reduction in waste generation, ensure the obedience of all necessary regulations and accelerating the production of innovative and sustainable packaging materials such as biobased materials, scavenging materials, active and intelligent packaging (Raja et al., 2023).

Modeling and simulation techniques for food packaging comprises three main domains: Deterministic chemical safety modeling, Mechanistic physics-based simulation and Stochastic environmental impact assessment (LCA). The deterministic chemical safety modeling and simulation helps to predict the migration pathways and predicts the shelf life of the packaged material. The mechanistic physics-based simulation helpful to optimize the fluid flow behavior, thermal conditions and mechanical performance of the package while the stochastic environmental impact assessment helps to quantify and improve the sustainability of the packaging materials.

The migration of compounds such as chemicals, toxicants, water vapour, antioxidants etc. is a problem in packaging. Migration leads to deterioration of the quality of the product as well as possess the health risks for the consumers. The migration of the chemicals depends on the environmental factors such as temperature, humidity, pH etc. The problem of migration generally arises during non-monitored storage and transportation (Seref & Cufaoglu, 2025). The mathematical modeling for migration analysis provides an easy, rapid and accurate method of detection. Fick's law and kinetic models are important to analyse the migration. Weibull model is a computational program which uses Fick's law for analysing the migration in a system (MARIA F. POÇAS, JORGE C. OLIVEIRA, RAINER BRANDSCH, 2011).

The design structure plays an important role in marketing, protection and preservation of the food products. Rigidity and flexibility of the packaging materials help in predicting the impact of loads and stresses during the processing, storage and transportation. Also, design of packaging material and type of material used are important parameters in maintain the required internal atmosphere of the system. The traditional 'trial and error' method gives less accuracy. Advanced modeling and simulation tools such as CFD and FEA are beneficial for studying the strength of package, fluid flow, heat transfer virtually. CFD model is used to solve problems related to fluid flow, mass transfer, heat transfer and chemical reactions. It gives the freedom of analyzing any location of the system under hypothetical situations. CFD is known for generating accurate analysis results (Szpicier et al., 2023a). FEA modeling and simulation techniques is used to analyse the impact of the load and stress. It can be used to check the heat transfer and mass flow in the package. Both the techniques several mathematical equations and computational tool to analyse the system (Fadiji, Berry, et al., 2018).

Food packaging is one of the necessary parts of food industry, but it is also responsible for generating a lot of waste. LCA cycle is used to analyse the shelf-life property of the food product as well as packaging materials. It also uses mathematical models and computational models for analysing the shelf life (Gao et al., 2025). The modeling and simulation techniques are advanced than traditional approach of creating a food package. However, integrating all three of the modeling and simulation methodologies discussed has received very little attention when it comes to building a substantial food packaging material. By providing a thorough analysis of each of the three modeling and simulation approaches, this paper seeks to close the gap. The mathematical formulas used to analyse the package's migration properties will be discussed at the start of the review. Next, using pertinent examples, we will talk about mechanistic and stochastic modeling and its methods, such as computational fluid dynamics and finite elemental analysis. Lastly, we will wrap up the review by talking about the difficulties and potential developments in food packaging.

3. Deterministic chemical safety modeling (migration)

Deterministic chemical safety modeling focuses on the mass transfer in a package occurring because of the interaction between the food product and the packaging materials and the impact of the environment factors such as temperature, humidity etc. The mass transfer phenomena are known as migration. It is a diffusion driven transfer process which promotes the migration of harmful chemicals, plasticizers, inks, additives and valuable antioxidants, vitamins, phenolic components, etc. This leads to contamination and spoilage of food and can cause health problems. Migration also affects the quality of packaging material and decreases the barrier properties, strength and shelf life of packaging material. The migration is of two types: Global and specific. The migration of all chemicals from packaging material to food is known as global migration whereas migration of a distinct and recognizable chemical compound is known as specific migration. Though migration is temperature-time dependent process and starts under specific time and temperature but there are other factors such as characteristics of packaging material, composition of food, period of contact, etc. which influence the initiation and rate of migration (Gupta et al., 2024a).

Migration model can be described as the process of analyzing the dynamics/flow of chemicals, vapours, particles between food and a packaging material. It is important to predict the shelf life of food products under various conditions. Usually, mathematical approaches are used to calculate the migration properties of a package (Gavril et al., 2018). Migration is governed by two phenomena: partition and diffusion. The partition coefficient gives a relation between concentration of migrants in packaging and food phase at thermal equilibrium (Gupta et al., 2024).

$$k = \frac{C_{PM}}{C_{FP}}$$

where, K = partition coefficient, C_{PM} = migrant equilibrium concentration in the packaging material and C_{FP} = migrant equilibrium concentration in food phase

The diffusion model governs the migration of molecules when it takes place from higher concentration to lower concentration till, they attain the state of equilibrium. Fick's First Law of Diffusion is used to explain the diffusion phenomenon. It provides a steady-state relation between the diffusive flux and the concentration gradient (Gupta et al., 2024):

$$J = D * \frac{\Delta C}{L}$$

where, J = Diffusive flux of permeant through perforation ($\text{mol.m}^{-2}.\text{s}^{-1}$), D = Diffusivity ($\text{m}^2.\text{s}^{-1}$), ΔC = Difference in concentration of permeant across packaging (mol.m^{-3}) and L = Path length (m)

Fick's first law of order is used when the diffusion takes place through larger pores i.e. pores having diameter larger than 1×10^{-5} m whereas for packaging material's having diameter lesser than 1×10^{-7} m, Knudsen Law is used for analysis of diffusion:

$$J = 48.5 \frac{d}{RTL} \left(\frac{T}{1000M} \right)^{0.5} \Delta p$$

where, d = Diameter of perforation (m), R = Ideal gas constant ($8.314 \text{m}^3.\text{Pa.K}^{-1}.\text{mol}^{-1}$), M= Absolute temperature (K), T = Molecular mass of diffusing gas (kg.mol^{-1})

The concentration of gases continuously changes with time in a food package. Hence, Fick's first law cannot be successfully used for the analyzing the migration. Fick's Second Law of diffusion is used to analysis the migration under unsteady state conditions:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left(\frac{D(C) \partial C}{\partial x} \right)$$

where, C = Concentration of permeant (mol.m^{-3}), D = Spatial position in x-direction (m), X = Diffusivity ($\text{m}^2.\text{s}^{-1}$)

3.1. Applications for Migration Modeling

The deterministic modeling is helpful in identifying the migration of potential risky elements in packaged material. Food contact materials (FCM) are the primary concern of human health. The migration modeling helps to improve the packaging design to prevent migration and to discard the risky element. A lot of research has been done to analysis the migration rate in food packaging. Forooghi et al., 2022, studied the migration of Irganox 1010, Irganox 1076 and titanium dioxide from laminated film to fermented milk-dough and acetic acid 3% at different storage conditions (time-temperature). they found that migration of chemicals was low (safe limit) and occurred only at some specific storage conditions. Irganox 1010 and TiO_2 migrated into dough. The highest concentration of Irganox 1010 was 0.8 ± 0.04 mg/l in acetic acid 3% (w/v), while 0.62 ± 0.04 mg/l in Dough. TiO_2 migrated in low concentration and was found to be 0.25 ± 0.04 mg/l in acetic acid 3% (w/v), and 0.12 ± 0.02 mg/l in Dough. POÇAS et al., 2012 used mathematical models, fick's law and Weibull distribution model to study the migration rate of toxic metals from the plastics, recycled paper and board into. They found that the fick's failed to analyse the migration during lag phase whereas Weibull model worked effectively over time.

4. Physics Based Modeling (FEA and CFD)

Physics based models are used to analyze the effectiveness of food packaging materials to bear the tension from continuous heat and mass transfer, stress and mechanical impacts during transportation. They follow fundamental physic laws such as Fourier law of heat transfer, hooke's law, fick's law for mass transfer, bernoulli's equation, boundary value problem etc. These laws are known for generating precise and measurable results (Datta, 2008). The application of physics law for calculation of heat and mass transfer is a time-consuming process. There are different computer softwares available which use physics law for analysing the system virtually. Later, the results can be used for designing of the real models (Datta, 2008). Finite Elemental Analysis (FEA) and Computational Fluid Dynamics (CFD) are two important modeling and simulation tools used for virtual testing of the system.

4.1. Finite Elemental Analysis (FEA)

FEA is a physics based computational simulation method which is used for studying the structure and problems of the system. It uses boundary value problems and continuity equations to study across multiple interconnected small and simple regions like squares, triangles etc. The results are later combined to validate the accuracy of the results (Fadiji, Berry, et al., 2018). FEA is widely used for food packaging to check the functionality, integrity and safety of the packaging throughout the cycle. It offers multiple advantages and helpful in optimal packaging design (Lim & Kim, 2023).

FEA uses the concept of piecewise polynomial interpolation. Here, instead of analysing the whole system in one operation, the system is divided into small finite units. The calculation is done across each unit, and results are later combined to produce the result for the entire system.

$$[K]\{u\} = \{f\}$$

where, $[K]$ = elementary stiffness matrix, $\{u\}$ = vector of the unknown nodal displacements (or temperature in thermal analysis), $\{f\}$ = vector of the applied nodal forces (or heat flux in thermal analysis)

FEA consists of three major steps: pre-processing, analysis and post-processing.

4.1.1. Pre-processing

This is the first step of FEA simulation where a model of the system is generated using computer programs like computer aided design (CAD). After generation of the model, the mesh is generated. A mesh is a discretized structure which is created by dividing the system into sub-regions known as elements and are connected through nodes. All the analysis and calculations are done at nodes only, e.g. calculation for analyzing the stress will be done on nodes only (Fadiji, Berry, et al., 2018).



Fig 1: A beverage bottle showing mesh structure for FEA modeling

4.1.2. Analysis

It is the processing stage where a computer simulation model known as Solver is used to solve mathematical equations across the nodes. After the mesh generation, the input values (load, mechanical properties, heat, geometry etc.) are put into finite element code to equations. The calculation analysis across each node generates a matrix. These matrixes are then reassembled to generate a global matrix which represents the entire system considered for analysis (Fadiji, Coetzee, et al., 2018).

4.1.3. Post-processing

After the analysis, all the data is combined and evaluated and used to create a virtual representation of the system either in 2D or 3D model. Different colours can be used to show the deformities in the package (Fadiji, Coetzee, et al., 2018). For example, red colour is used to show plastic deformation zone in the aluminium can.

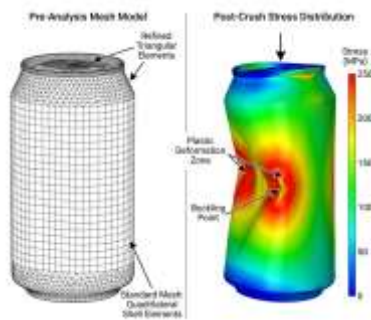


Fig 2: Finite element analysis of a beverage can tester

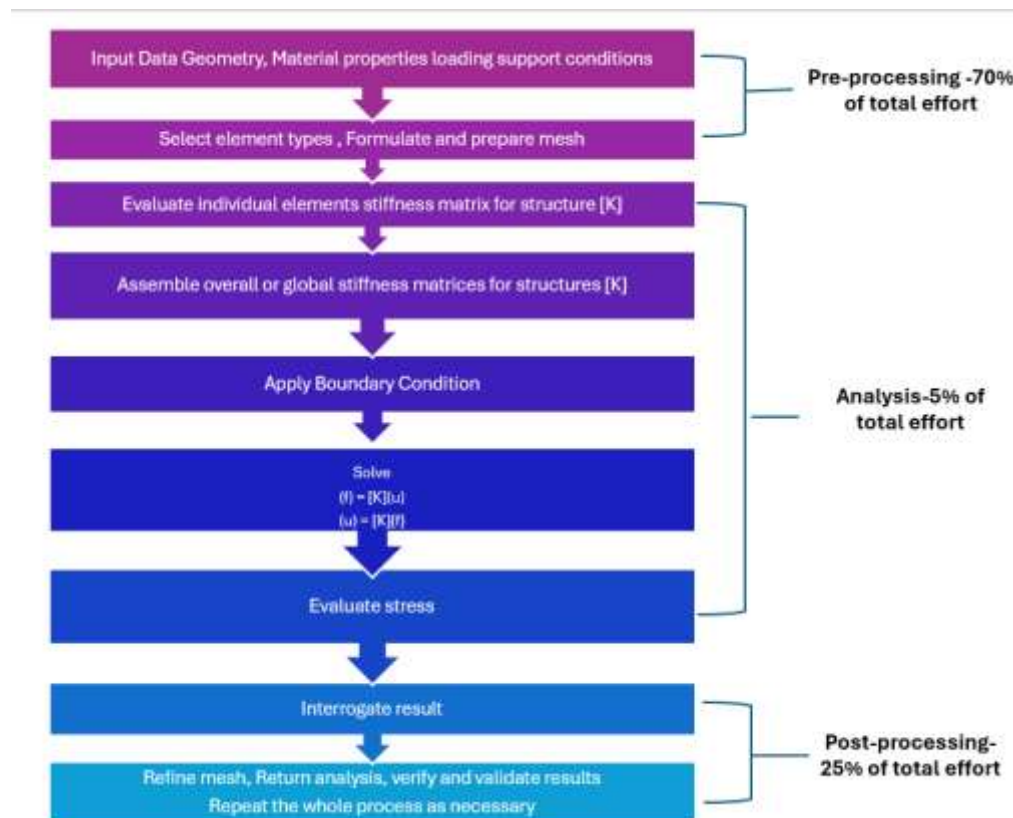


Fig 3: General Steps to proceed Computational Analysis in FEA

4.1.4. Softwares for FEA modeling in food packaging

Several softwares are used for FEA modeling in food packaging. The selection of a software depends on the needs of the engineer, complexity of the system, properties of the materials and required geometry of the package. Some of the tools are described in the table below:

Table 1: List of FEA software

FEA software	Description
ANSYS Mechanical	It uses Multiphysics integration, supports high-performance computing and can be used for large and detailed simulations.
Abaqus (SIMULIA)	It is commonly used for non-linear analysis and simulation of complex material behaviour such as plastic deformation, elastic behaviour. It can be combined with other modeling techniques also such as CAD.
MSC Nastran	It is a type of FEA solver which is effectively used for analysis of larger structures.
COMSOL Multiphysics	It is a kind of equation-based approach where users can write their own equations to solve the structure and migration related problems.

4.1.4. Applications of FEA

FEA is mainly used in the food packaging industry for designing of the packaging and analysing the performance under different conditions. Yuan et al., 2013) optimized the design conditions using ANSYS FEA software. They analysed the strength of the PET bottles having different thickness and diameter for checking internal pressure using the computational model. (Li et al., 2013) analysed the deformation in three and four locular tomatoes under compressive force. The multiscale FEA analysis showed that maximum damage was caused when the four locular tomatoes were compressed at a position midway. (Vatankhah et al., 2015) optimized the thermal processing conditions of Haleem in aluminium containers. The model identified the slowest heating zone at the centre of the can. The heating time for centre part was observed about 23 minutes. It was also found that interval heating of the can helped to reduce the time.

4.2. Computational Fluid Dynamics (CFD)

CFD is a computational tool for modeling and simulation which is mainly used for governing the fluid flow across a system using mathematical equations. It integrates the fluid flow, mathematics and computer science. Where computer codes are used to solve the problems mathematical equations of fluid flow, thermal and mechanical processes. This allows researchers to do multiple analysis at a time. It takes less analysis time than other empirical analysis techniques (Szpicer et al., 2023b). CFD is more advanced technique than FEA for calculating the fluid flow across the system.

The CFD modeling and simulation follows the same steps for analysis like FEA i.e. pre-processing, processing/analysis and post-processing. A no. of mathematical equations are used for calculating the fluid flow in a system such as Newton's law of motion, Bernoulli's equation, continuity equation, boundary value theorem. Navier-stokes equation is the basic equation for CFD modeling. Specialized software tools are used to solve the mathematical equations and execute the program (P, Abhinash, Dhanya Suresh, 2024).

4.2.1. Pre-processing

The CFD process starts with formulation of problem, mesh generation and creation of CFD model. This step is also known as equation discretization. The entire is discretized into finite elements. Before making the CFD model, engineers analyze the problems and verify the intrinsic areas where flow can take place. They enlist all the possible mathematical equations to gain knowledge about the system. After formulating the problem, using software tools a mesh is developed same like in FEA analysis. Nodes, elements and degree of freedom are defined across the mesh.

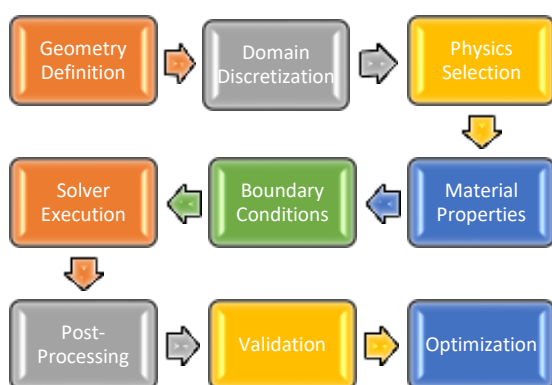


Fig 4: Systematic presentation of CFD analysis

4.2.2. Processing

In this step, a solver is chosen to solve all the mathematical equations. The solved data for each element is integrated several times to generate a reliable result (Szpicer et al., 2025).

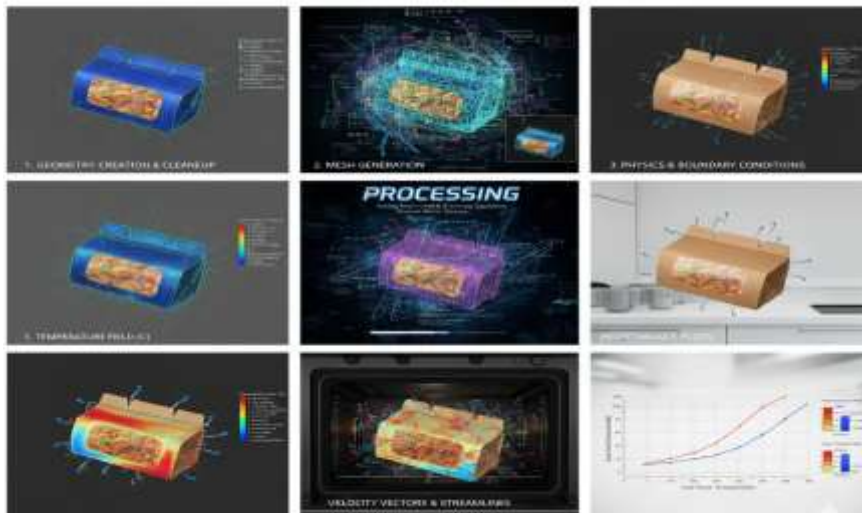


Fig 5: CFD analysis across a food package

4.2.3. Post-processing

After all calculations, the results are combined and verified. The iteration of the data generates a reliable output for the whole system. These data can be represented into either into 2D or 3D design using different CFD softwares (P, Abhinash, Dhanya Suresh, 2024).

4.2.4. CFD analysis softwares

The selection of softwares depend on the complexity of the system, package application and availability of the resources.

Table 2: Softwares for CFD modeling

S.No.	Software Package	Primary Advantage in Food Packaging
1.	Ansys Fluent	High-performance, industry-standard solver.
2.	COMSOL Multiphysics	Seamless coupling of multiple physical fields.
3.	OpenFOAM	Open-source flexibility and customization.
4.	M-Star CFD	Real-time Dynamics on GPUs.

4.2.5. Application of CFD in Food Packaging

CFD can be applied for studying various applications from basic heating and cooling systems to the modeling and simulation of the smart packaging systems. (Gaona-Forero et al., 2018) used CFD model for studying the moisture adsorption by sodium polyacrylate (SPA) based adsorbers and moisture loss in Hass avocado packed in PET packages for 12 days at temperature of 12°C. The observed results were showed that CFD gave fast and more precise results when compared with mathematical models for analysing the same properties. Nasser eddine et al., 2025 used CFD model to develop a cardboard packaging material for strawberries. The packaging material was divided into two sections, each containing six spaces. The dividing part had holes for the flow of air. Two types of packaging were made, one with symmetrically aligned holes and other with asymmetrically aligned holes. The analysis showed that alignment of the holes played major role in mass transfer. The package with symmetrical holes observed to have more colling effect. (Zhang et al., 2022) modelled a package for keeping Covid vaccines at freezing temperatures using CFD modeling. They incorporated the insulating materials and reduced barrier for fluid flow. They analysed that by varying the type and thickness of insulating material and reducing the hinderances for air-flow helped in maintain the temperature at low level.

4.3. Advantages and disadvantages of FEA and CFD modeling

Advantages:

1. It helps in cost reduction.
2. It accelerates the development cycle.
3. It enhanced the quality of the final product.
4. It helps in achieving sustainability.
5. It can be easily incorporated with other designing tools.

Disadvantages:

1. The computational operation is a complex process, and it needs an expert for the analysis.
2. Modeling and simulation results need validation.
3. It is tough to model multilayer structures using FEA and CFD.
4. Different FEA and CFD software are needed as per the complexity of the material and system.

5. Stochastic Life Assessment Modeling

Packaging is an important part of the food industry. Various kind of packaging materials such as paper and paperboard, glass, metal and plastics are used. It is essential to protect the food from environmental factors like moisture, gases, pests, insects etc. Though, packaging improves the shelf life of food products, but it also has a negative impact on the environment. It causes, creates landfill problems, pollution from manufacturing as well as disposal, emits Green-House-Gas (GHG) on manufacturing and combustion and disturbs the natural flora and fauna (Hemachandra et al., 2024). Plastic is the non-biodegradable and serves as the main culprit among all packaging materials. The virgin plastics are single used plastics and creates pollution land, water and water bodies after its use. These negative impacts create necessity for the development of biodegradable materials using renewable sources and a method to check the product's sustainability (Yadav et al., 2024).

The Life Cycle Assessment (LCA) modeling is method to measure the sustainability of the packaging materials. The ISO standard defines LCA in several ways. ISO 14040 defines the principles and frameworks of LCA whereas ISO 14044 focuses more on requirements and guidelines for LCA. LCA leads to the way of sustainable packaging supporting by generating effective outputs for supporting the decision-making process (Bremenkamp & Sousa Gallagher, 2024). It is most used tool to analyse the impact of packaging materials on environment and supports decision making and policy making. LCA studies the life cycle of a package around the supply chain. This method is mainly used for assessing, quantification and comparison of the impacts of product on environment and suggest how many times a reusable container can be used (Yadav et al., 2024). It comprises a series of questions specifically for the product or process which can contribute to the food waste (Hemachandra et al., 2024).

According to ISO 14040, LCA can be divided into four interrelated steps (Bremenkamp & Sousa Gallagher, 2024):

5.1. Goal and scope definition

It defines the aim of the process; functional units need to define the process e.g. mass or volume of the product, system boundaries from starting of the production till the end use, impact categories for the analysing the effect of environmental factors on product and geographical scope of the opted method.

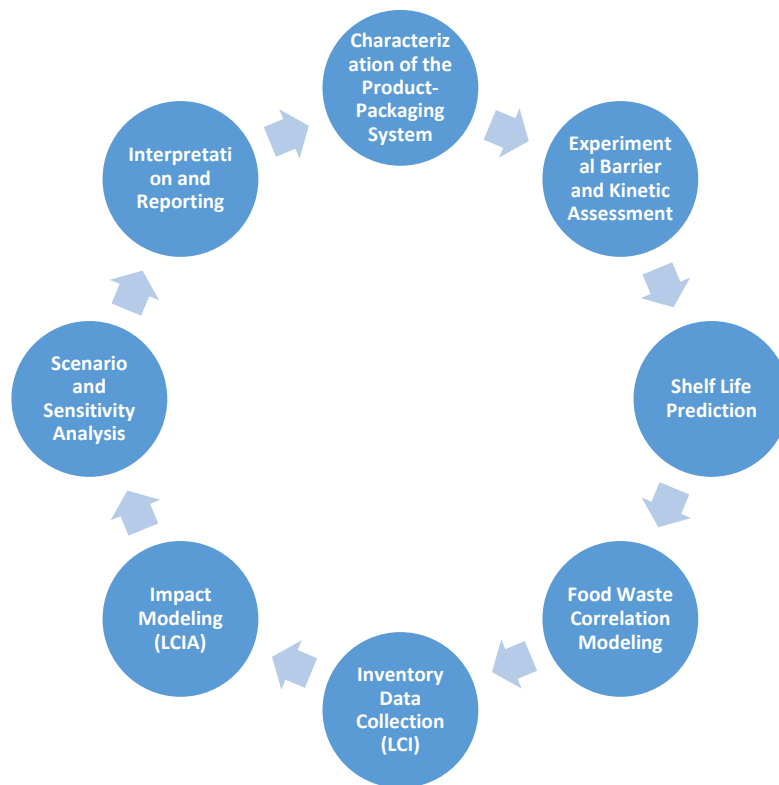


Fig 6: Flowchart for Proceeding with a Food Packaging LCA

5.2. Life Cycle Inventory Analysis (LCI)

This step deals with collection of data at every input (energy, raw materials) and output point (emissions of air, water etc.). The LCI data is important to predict the impact of various factors on the shelf life e.g. the antibacterial agents in a package enhance the shelf life of food product.

5.3. Life Cycle Impact Assessment (LCIA)

It is helpful in converting the collected LCI data into meaningful and related environmental impacts.

5.4. Interpretation

It analyses the data from all the three steps, concludes the process and give recommendations for improving the process.

5.5. LCA Models for predicting the Shelf Life

The shelf life of food product as well as the packaging greatly depends on the interaction between two and the impact of environment. Mathematical models used for analysing the migration (Fick's second law of diffusion), models for analysing mass transfer and permeability (Fick's first law of diffusion), kinetic modeling for analysing the shelf life (zero-order, first order and second order kinetic model), and model for analysing the change in temperature (Arrhenius model) are used.

5.5.1. Water activity (a_w)

Water activity is used to measure the amount of free water present in the system. This free water supports the growth of micro-organisms, promotes enzymatic activity which ultimately leads to the spoilage of food products. Water activity can be defined as the ratio of partial pressure of water vapor (p_i) in the product to the partial pressure of pure water (p_0) (Mathlouthi, 2001).

$$a_w = p_i^{H_2O} / p_0^{H_2O}$$

where, a_w = Water activity, $p_i^{H_2O}$ = Vapour pressure of water exerted by the system (Pa), $p_0^{H_2O}$ = Saturated vapour pressure of pure water at the same temperature (Pa)

a_w is a crucial indicator of shelf-life stability. It ranges from 0 to 1. Higher activity ($a_w > 0.95$) supports the growth of bacteria, yeast and mold and cause spoilage of food products.

5.5.2. Arrhenius Model

During storage and transportation, food products bear a great change in temperature which affects their quality and reduces the shelf life. The Arrhenius Model is used to check the temperature sensitivity of the product (Bunkar et al., 2014a).

$$k = Ae^{-\frac{E_a}{RT}}$$

Where, k : Rate constant of the reaction, A : Pre-exponential factor, which is related to the frequency of collisions and their orientation, E_a : Activation energy, the minimum energy required for a reaction to occur, R : Universal gas constant, $8.314 \text{ J/mol} \cdot \text{K}$, T : Absolute temperature in Kelvin

5.5.3. Kinetic Modeling

Kinetic modeling is a method of developing mathematical equations of chemically reacting system. The modeling helps to calculate the rate of reaction for a change in attribute of a particular component. For example, the change in sugar composition during ripening can be modelled and calculated using kinetic modeling (Bunkar et al., 2014).

$$-\frac{d[A]}{dt} = k[A]^n$$

where, A = concentration of the attribute, t = time, k = reaction time constant, n = order of the reaction

There are three orders of chemical kinetic modeling to check food spoilage:

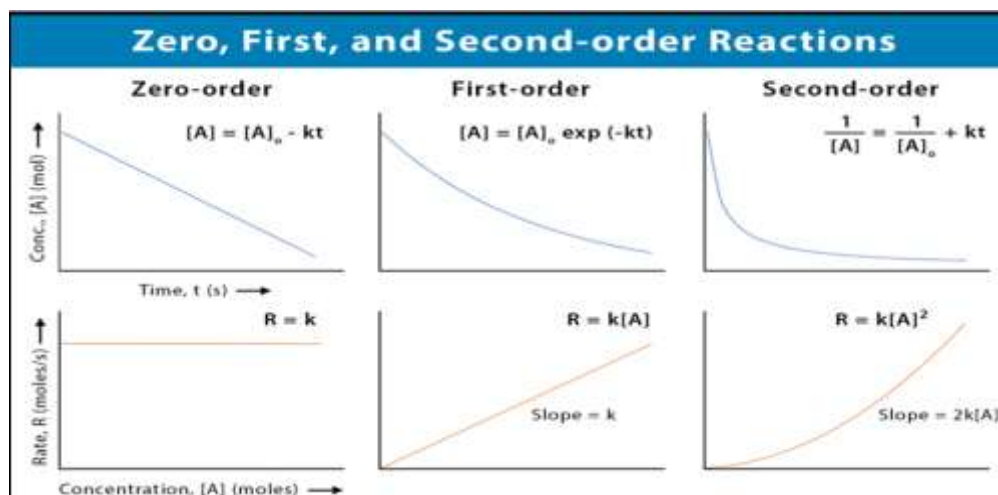


Fig 7: Zero, First and Second order kinetic reactions

1. Zero order kinetic model (here, $n = 0$, which means the rate of change of reaction is independent of the concentration of the attribute)
2. First order kinetic model (here, $n = 1$, which means the rate of change of reaction is directly proportional to the concentration of the concentration of the attribute)
3. Second order kinetic model (here, $n = 2$, which means the rate of reaction depends on the interaction of two components)

5.6. Applications of LCA in food packaging industry

The LCA cycle performs the comparative analysis between the developed package and the existing materials or sometimes between various types of materials and systems to check their their impact and sustainability in the

environment. Yadav et al., 2024 studied the LCA cycle of a reusable polypropylene takeaway container for food for checking the effects multiple usage to the single-use container. They found that the global warming potential (GWP) was significantly decreased after each use. GWP for single-use container was 1.3 times higher ((0.020 kg CO₂ eq./FU) than container used for 10 times (0.015 kg CO₂ eq./FU). 100 uses resulted in 83% reduction (0.007 kg CO₂ eq./FU) in GWP. Stramarkou et al., 2022 compared the LCA cycle of a smart food packaging (SP) system (encapsulated oregano essential oil (OEO) into LDPE matrix) and equipped with a chemical sensor with a conventional packaging material. They observed that the development of SP had 67% impact on climate change and generated only 5% (optimistic), 10% (realistic) and 20% (conservative scenario) waste, whereas around 30% waste was generated by CP after four uses and EoL consequences. (Eslami et al., 2025) studied the impact of recycling the packaging materials used for peeled tomatoes and tomato puree. The EoL data showed a significant reduction in CO₂ emissions i.e. 46% and 48% for recycled metal and glass packaging materials respectively in comparison to single-use metal cans and glass bottles which were responsible to generate 0.666 kg CO₂eq and 0.479 kg CO₂eq, respectively.

5.7. Advantages and disadvantages of LCA Modeling in Food Packaging

Advantages of LCA

1. It helps in identification of the points where the most significant damage can occur.
2. It helps in contributing to sustainability of packaging without effecting the other processing areas.
3. It maintains a correlation with the regulatory bodies by providing a justification and proofs for environmental claims.
4. LCA promotes circular economy by promoting the recyclability and use of sustainable packaging materials.
5. It is flexible to use with ISO regulations and allow to use select model type as per user choice.

Disadvantage of LCA

1. LCA modeling primary data at each step of supply chain which is quite difficult to obtain. Assumed hypothesis and data results in inaccurate results.
2. LCA modeling is a complex, time consuming process. Different softwares such as SimPro and GaBi are needed to do the modeling.
3. Usage of multiple models for LCA analysis creates conflicts as there is no universally accepted model available for predicting the shelf life of the products.
4. The flexibility of the system greatly influences the end results and biasness.

6. Discussion and Conclusion

Modeling and simulation have revolutionized modern food packaging design by enabling data-driven, efficient, and sustainable solutions. These techniques integrate chemical, physical, and environmental analyses to optimize package performance, safety, and longevity while minimizing material use and ecological impact. By replacing traditional trial-and-error methods, modeling tools not only reduce development costs and time but also improve prediction accuracy. However, their successful implementation depends on precise data input, robust computational models, and expert interpretation. As the food industry continues to evolve, the integration of these advanced modeling approaches will play a central role in achieving smart, safe, and sustainable packaging innovations.

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