Imperial College London

Department of Earth Science and Engineering

MSc in Applied Computational Science and Engineering

Independent Research Project

Project Plan

Predictive Modeling of Shelf Life for FMCG Snack Products

by

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June 2025

Abstract

Shelf-life prediction for snack products is a critical challenge in the highly competitive FMCG sector, where product quality is influenced by multiple degradation mechanisms. Moisture gain and lipid oxidation are two key pathways affecting product stability, yet they are often studied independently. Moisture behaviour is often described using the Guggenheim-Anderson-de Boer (GAB) model together with moisture transfer equations, while lipid oxidation follows temperature-dependent kinetic models based on Arrhenius principles. However, their interaction, particularly the impact of water activity on oxidation rates, remains underexplored. The goal of this project is to develop a coupled computational model that integrates both moisture and lipid oxidation effects to estimate shelf life more accurately, providing valuable insights for product development and packaging design.

1. Introduction

The snack food segment of the Fast-Moving Consumer Goods (FMCG) industry is highly competitive; thus, maintaining product quality is not only expected but necessary. Predicting shelf life is crucial in different aspects, from consumer satisfaction to inventory management. For snack products, which often undergo quality degradation due to moisture gain and chemical deterioration, particularly lipid oxidation, having a reliable method to estimate shelf life is not just helpful but essential to avoid spoilage, reduce waste, and support timely distribution.

Over the years, a number of mechanistic models have been developed to address the spoilage pathways. Research on predicting shelf life limited by moisture gain is well established, with Moisture Sorption Isotherm (MSI) models forming the foundation of most approaches. These models describe how a product's moisture content relates to its water activity (a_w), a key factor in determining textural stability [1; 2]. The Guggenheim-Anderson-de Boer (GAB) model is one of the most widely used due to its flexibility and strong fit across a broad water activity range [3; 4]. Its parameters also offer physical interpretability, such as the monolayer moisture content (m_0), which is often considered a critical point for stability. As a result, the GAB model is frequently used in shelf-life predictions for packaged low-moisture foods. Simpler linear MSI models have also proven effective and can offer comparable accuracy in the low water activity ranges typically observed in crispy snacks [5]. These models are often used to estimate the time required to reach a critical water activity or moisture content level, which is closely tied to sensory attributes like crispness.

In parallel, shelf-life predictive modelling for lipid oxidation has received substantial attention, particularly for products containing fats and oils. Lipid oxidation leads to off-flavours and rancidity and is a major driver of quality loss [6; 7]. Predictive models are typically based on chemical kinetics and rely on Accelerated Shelf-Life Testing (ASLT) in this area, using temperature to accelerate deterioration [7]. Progress is monitored by tracking primary oxidation products (such as hydroperoxides) and secondary products (such as hexanal) [7; 8]. Kinetic behaviour is often modelled using pseudo-zero or first-order reaction assumptions, with temperature effects described by the Arrhenius equation to derive parameters like the rate constant (k), activation energy (E_a), and Q_{10} value [7; 9]. Some studies extend this with Eyring-Polanyi equations to incorporate thermodynamic parameters or apply multi-phase models to capture more complex reaction stages, such as initiation, propagation, and secondary acceleration phases [8; 9; 10].

While both moisture-driven and lipid oxidation-driven shelf-life predictive models are individually well developed, they have typically been applied separately. However, both mechanisms may simultaneously occur and not be entirely independent in some FMCG snack products—most notably, the influence of water activity on the rate of lipid oxidation [7]. Although some studies monitor water activity alongside oxidation during ASLT, few approaches couple the two processes within an integrated predictive model. This project seeks to address that gap by developing a coupled shelf-life prediction model which accounts for the interdependence of these mechanisms. The goal of the model is to improve predictive accuracy and offer valuable insights for packaging design, product development, and shelf-life extension in the FMCG sector.

2. Methodology

2.1. Mathematical Models

This project models shelf life in snack products by focusing on two dominant degradation pathways: moisture gain and lipid oxidation.

2.1.1. Modelling Based on Moisture Gain

One aim of this project is to solve the equation that defines the shelf life of the product:

$$t_{s,\text{moisture}} = \int_{a_{w0}}^{a_{wc}} \frac{W_s \cdot L \cdot S(a_{w,\text{food}})}{P_w \cdot A \cdot p_0 \cdot (a_{w,\text{env}} - a_{w,\text{food}})} \, da_{w,\text{food}} \tag{1}$$

This integral represents the time required for the food's water activity to increase from its initial value a_{w0} to a critical threshold a_{wc}, beyond which product quality is compromised. The function $S(a_{w,food})$ represents the slope of the sorption isotherm and is typically derived from the GAB model:

$$w = \frac{W_m \cdot C \cdot K \cdot a_w}{(1-Ka_w)(1-Ka_w+CKa_w)} \tag{2}$$

Moisture transfer through packaging is modelled via a one-dimensional form of Fick's law, incorporating packaging parameters like water vapour permeability (P_w), surface area (A), and film thickness (L). The rate of a_w change within the product is expressed as a function of the environmental $a_{w,env}$, food product $a_{w,food}$, and $S(a_{w,food})$ at the current state:

$$\frac{da_{w,\text{food}}}{dt} = \frac{P_w \cdot A \cdot p_0}{W_s \cdot L \cdot S(a_{w,\text{food}})} \cdot \left(a_{w,\text{env}} - a_{w,\text{food}}\right) \tag{3}$$

2.1.2. Modelling Based on Lipid Oxidation

Lipid oxidation is modelled as a temperature-dependent reaction, following pseudo-zero or first-order kinetics. The Arrhenius equation is used to describe how the reaction rate varies with temperature, with key parameters including the activation energy (E_a) and pre-exponential factor (Z):

$$k_{\text{ox}} = Z \cdot e^{-E_a/(R \cdot T)} \tag{4}$$

2.1.3. Combined Predictive Model

The overall shelf life is defined as the minimum time at which either the critical a_w or a critical oxidation marker is reached. If interactions are significant, a coupled kinetic model will be used, where $a_w(t)$, derived from the moisture transfer model, regulates the oxidation rate dynamically.

2.2. Numerical Implementation

The system of ordinary differential equations (ODEs) will be solved numerically using time-stepping methods, such as Runge-Kutta schemes, while shelf-life estimations will involve numerical integration, implemented in Python with the NumPy and SciPy libraries.

2.3. Validation Strategy

Model predictions will be validated against experimental data using curve fitting and error metrics such as RMSE and MAE. Sensitivity analysis will be used to assess the influence of uncertain parameters.

2.4. Deliverables

The final deliverable will be a computational tool capable of simulating the evolution of product quality and estimating shelf life under diverse scenarios.

3. Future Plan

The specific objectives for this project are:

3.1.To implement numerical methods for solving differential equations that describe the deterioration kinetics, such as moisture transfer and lipid oxidation.

3.2.To implement numerical integration methods for simulating the dynamic evolution of product quality under various environmental conditions.

3.3.To establish a comprehensive predictive model for product shelf life by integrating moisture-driven methods and lipid oxidation-driven methods.

3.4.To validate the kinetic model by comparing simulation outputs with experimental data from accelerated shelf-life tests.

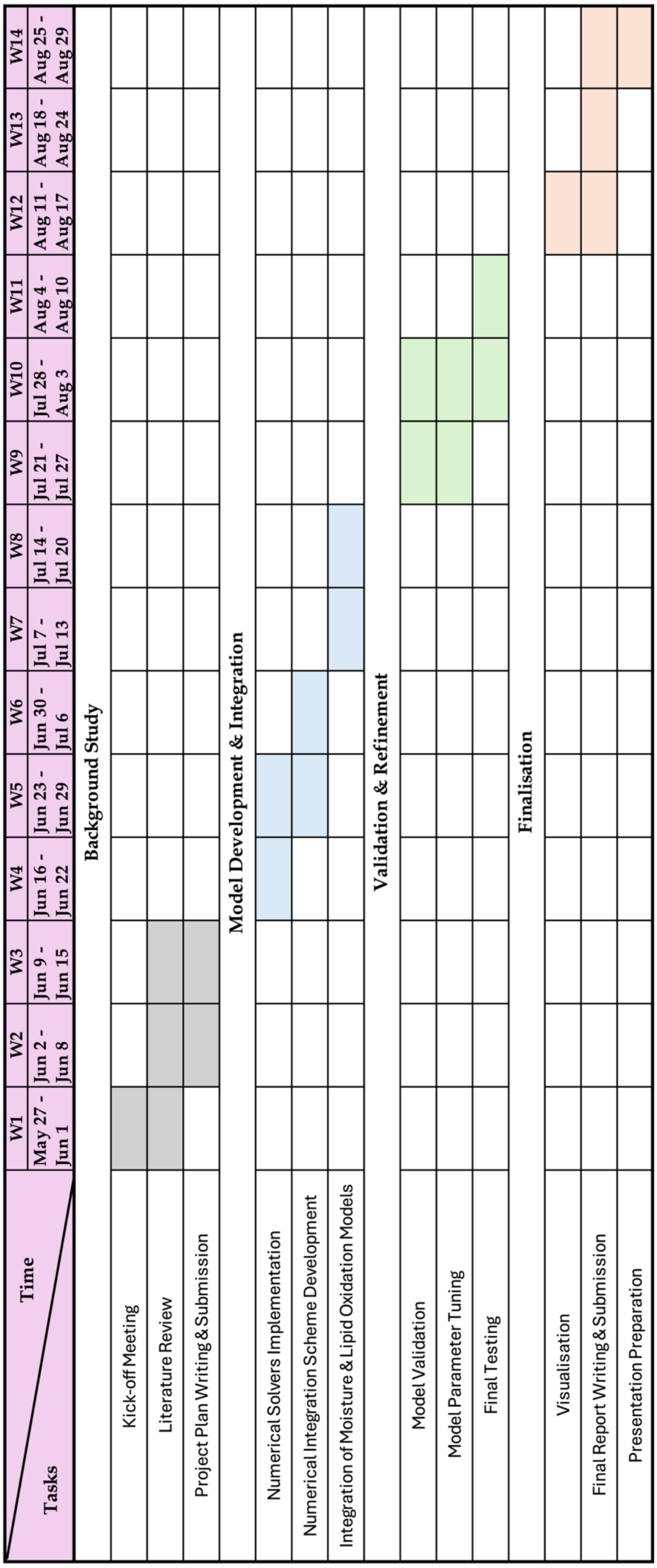

Figure 1: Project Gantt Chart

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Appendix

Symbol	Description
w	Equilibrium moisture content
a_w	Water activity
W_m	Monolayer moisture content
C	Guggenheim constant (related to monolayer binding energy)
K	Multilayer constant (related to multilayer water properties)
$\frac{da_{w,food}}{dt}$	Rate of change of food water activity over time
P_w	Water vapour permeability of the packaging material
A	Surface area of the package
p_0	Saturation vapour pressure of pure water at storage temperature
W_s	Mass of dry solids in the product
L	Thickness of the packaging film
$a_{w,env}$	Water activity of the external environment
$a_{w,food}$	Water activity of the food product
a_{w0}	Initial water activity of the food product
a_{wc}	Critical water activity at which the product is considered unacceptable
$\mathrm{S}(a_{w,food})$	Slope of the sorption isotherm at the current food water activity
$t_{s,moisture}$	Shelf life limited by moisture gain
k_{ox}	Rate constant of lipid oxidation
Z	Pre-exponential factor
E_a	Activation energy of the oxidation reaction
R	Universal gas constant
T	Absolute temperature

Table 1: Appendix