**DEVELOPMENT OF COMPUTER SOFTWARE FOR THE ANALYSIS OF DATA FROM AGRO PRODUCTS DEHYDRATION**.****

**Presented to**

**The Department of Chemical Engineering**

**By**

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**In Partial Fulfillment of the requirement for the Award of**

Bachelor of Science (B.Sc.) Degree

In Chemical Engineering

At The

UNIVERSITY OF LAGOS

# ABSTRACT

The dehydration of agro-products is an important process in food preservation. As a critical post-harvest process, it significantly extends shelf life and maintains the quality of the products. However, analyzing moisture ratio history data to determine drying kinetics, thermodynamic properties and thin-layer modelling remains a tedious task. Conventional techniques for analyzing dehydration data includes the use of spread sheets and manual calculations. While effective, these methods have several limitations such as time consumption, high risk of error, and limited automation. This research focuses on the development of a computer software designed specifically to analyze data from agro-products dehydration. The software written in python programming language takes moisture ratio history data as input, performs linear regression analysis to determine drying kinetics, thermodynamic properties and non-linear regression to fit defined thin-layer models to the data after which the results are exported to be saved on the user’s computer. Key features of the software include accurate computations, statistical evaluations of models, and comprehensive results. Validation was done using experimental datasets from existing dehydration research, confirming the software’s accuracy and reliability. This tool provides a practical and automated approach to analyzing dehydration data, offering significant benefits in agricultural and food processing research.

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# ****CHAPTER ONE: INTRODUCTION****

## Background of Study

One common method to preserve agricultural products is drying, in which moisture is removed by evaporation, and simultaneous heat and mass transfer occurs between the sample and the adjacent environment (Kamal et al., 2020). Drying is one of the most ancient and widely practiced techniques for preserving agro-products. It involves the removal of moisture to a level that inhibits the growth of microorganisms and enzymatic activity, ensuring the stability, safety, and longevity of agricultural products (Dhakal, 2022). As a critical post-harvest process, drying also reduces the weight and the volume of food products, which leads to a reduction in the expenses for packaging, storage and transportation.

Drying is an energy-intensive operation. It is estimated to consume 10% to 15% of the total energy requirements of all the food industries in developed countries (Onwude et al., 2016). According to Onwude et al (2016), dependence only on experimental drying data, without considering the mathematics of the drying kinetics, can significantly affect the efficiency of dryers, increase the cost of production, and reduce the quality of the dried product. Therefore, it becomes essential to apply mathematical models to estimate the drying kinetics, behavior, and the energy required to dry agricultural products.

One of the mathematical models used in the drying operation is the thin-layer drying model. BUZRUL described Thin-layer drying as the term used for the lumped systems for which a uniform temperature is generally assumed because of the thin structure of the fruit or vegetable that has been sliced before drying (Buzrul, 2022). Thin layer drying models are fundamental to drying simulation. Modeling the thin-layer drying of agricultural products is mainly based on describing the moisture ratio (MR) versus time (t) data using suitable mathematical models.

Fruits and vegetables are highly perishable commodities that needs to be preserved to increase shelf-life and their dehydration process can be predicted using suitable thin-layer models. Several researchers have studied the drying of fruits and vegetables using thin-layer drying models to estimate the drying time of a product (Onwude et al., 2016). Previous studies shows that these thin layer models can be used to Research indicates that these models can be applied to estimate the drying behaviour, heat and mass transfer, and energy consumption during the drying process (Murthy and Manohar, 2012). However, in reality, there is no single thin-layer model that can accurately represent the drying kinetics of various fruits and vegetables. This is due to the different drying conditions the product undergoes, the method of drying and the product itself (Onwude et al., 2016).

The use of thin-layer drying models to model the drying behavior of agro products often involves the measurement of the moisture content of the material and calculating the moisture ratio variation with time. This is done after it has been subjected to different drying conditions (temperature, air velocity, and relative humidity). Incorrect experimental data from the thin-layer dehydration experiments, will lead to incorrect moisture ratio history data and, subsequently, the selection of appropriate thin-layer models. Thus, the use of correct experimental data is a crucial step in using thin layer models to describe the drying behavior of agro products.

Due to the different thin-layer models available and the absence of a single thin-layer model that can be used to generalize the drying kinetics of agro products, it becomes necessary to carefully select the most accurate of these models. Traditional methods of analyzing dehydration data involves manual calculations and the use of generic tools like spreadsheets. While effective, these approaches have several limitations such as time consumption, error prone, and limited automation. The development of a specialized software can address these limitations by automating data analysis of dehydration data by accurately calculating the thermodynamic properties of the product such as enthalpy, entropy, Gibbs free energy, and activation energy. The most accurate thin layer drying model can also be calculated through; fitting of experimental moisture ratio data to various models, comparison of model’s performances using statistical indicators such as the coefficient of determination (R2), root mean square error (RMSE), and sum of squared errors (SSE).

## Aim and Objectives of Study

The aim of this research project is to develop a computer software for the analysis of data from Agro products dehydration. The Objectives of this research project includes:

1. To develop a computer software that accepts experimental dehydration data (moisture ratio and time) in an excel file format.
2. To implement methods for fitting the experimental data to several thin-layer models and determining model parameters.
3. To evaluate the performance of models using statistical indicators such as R² (coefficient of determination), RMSE (root mean square error), and sum of squared errors (SSE).
4. To accurately calculate the moisture diffusivity, activation energy, enthalpy, entropy and Gibbs free energy.
5. To display the results of these analysis in a csv file.

## Scope of Study

1. Conduct a literature review of food dehydration methods.

2. Conduct a literature review on the necessary calculations for food dehydration.

3. Conduct a literature review on methods for fitting data to model equations.

4. Develop software for analyzing dehydration data.

5. Evaluate the performance of models using statistical indicators.

6. Accurately calculate thermodynamic properties from dehydration data.

7. Package the software as an executable file for installation on any computer.

# CHAPTER TWO: LITERATURE REVIEW

## 2.1 Introduction

The dehydration of agro-products is a vital process in the agricultural and food industry, playing a critical role in extending shelf life, reducing transportation costs, and preserving nutritional value. Accurate analysis of data generated during dehydration processes is essential for optimizing drying conditions and ensuring product quality.

This literature review delves into the theoretical aspects of drying, focusing on mathematical modelling, experimental data interpretation, and data analysis. It begins by examining the fundamental principles of drying kinetics, highlighting the different thin layer models used such as Newton, Henderson-Pabis, and Page’s models. This literature also highlights the role of regression analysis in the integration of experimental data with predictive models, facilitating parameter estimation and the use of statistical parameters for the evaluation of the performance of the different models effectively.

## 2.2 Historical Review of Drying

For ages, people have used drying, mostly to preserve food and agricultural goods. Drying has been utilized for many other equally significant functions in modern times, even if its primary goal has been constant since its inception. Using drying to create goods that are impossible to obtain through other processing methods is one of these uses. This includes commonplace items like coffee, milk, and other drinks, as well as domestic goods like detergent powder and certain cutting-edge materials like medications (Devahastin & Jinorose, 2020).

Humans began using the sun to dry meat as early as 20,000 BC. While grains and legumes were dried in the Middle and Near East, fish was noted to be dried in France some 10,000 years later. Salt was created by drying saltwater around 9000 BC, while sugar was not dried into a solid state until 1500 years ago in India (Hayashi, 1989). The development of most drying techniques that are widely in use today started only in the nineteenth century. Around 1800, an early version of a mechanical dryer made of brick was constructed and used to dry grains.

In 1856, a method for concentrating and preserving milk by "coagulating and rearranging the albuminous particles in combination with the evaporation of the fluid in vacuo." Was patented by Gail Borden Jr. This method was based on his prior experience making the so-called meat biscuit (Borden, 1856), which was a dehydrated meat mixed with flour. This was an early attempt to create a vacuum-based water removal method. Since then, numerous additional patents on the manufacturing of different dried goods have been submitted. Charles A. La Mont, for instance, patented a method of producing dried eggs in 1865 (La Mont, 1865).

Freeze drying is another crucial drying technique, particularly for items as heat-sensitive as pharmaceutical products. It was initially discovered that Japanese monks living on a mountain used a method similar to freeze drying to dry tofu and that the Incas of Peru also used it to dry potatoes and other crops. In these situations, drying materials were transported high into the mountains, where temperatures dropped below the freezing point of water. Because of the high elevations and low atmospheric pressure, the water in the materials was removed (Hayashi, 1989). However, modern freeze drying did not begin until the late nineteenth century, when Richard Altman dried pieces of frozen tissues in a vacuum desiccator set at -20°C in 1890. During World War II, freeze drying gained popularity as a way to preserve blood plasma, vaccinations, and several other biological substances (Couriel, 1980).

With the advent of industrialization in the 19th century, drying technology evolved significantly. The development of mechanical dryers such as drum dryers and cabinet dryers, marked a shift from traditional methods to controlled drying processes. These innovations provided better control over drying parameters like temperature and humidity, improving the efficiency and quality of the drying process.

## 2.3 Basic Theory of Drying

The process of removing a relatively small amount of water or other liquid from a solid material in order to attain a sufficiently low residual moisture content is generally referred to as drying. It is usually the final step in a series of operations, and the product from a dryer is often ready for final packaging (McCabe et al., 1993, pp. 767).

A dried substance's liquid content varies from product to product; sometimes, a product is bone-dry, meaning it has no liquid. More commonly, the product contains some liquid in it. For instance, there is roughly 0.5 percent water in dry table salt, 4 percent in dried coal, and 8 percent in dried casein. According to McCabe et al. (1993, pp. 767), drying is a relative phrase that simply refers to a decrease in liquid content of a material from an initial value to a final tolerable value.

The primary goal of drying is to extend the shelf life of food materials. By lowering the moisture level, water activity is decreased, which lowers enzymatic activity, prevents microbial growth, and slows down the development of unwanted chemical reactions (Delgado & da Silva, 2014). In certain cases, drying enhances the organoleptic properties of food, making it more visually appealing to consumers. Examples include dried fruits, nuts, vegetables, and many other snacks, as well as specific types of meat or fish (Delgado & da Silva, 2014).

Due to the loss of water from, the mass of the material reduces giving the dried product less weight and a smaller volume when compared to fresh one, which makes it easier to package and transport, factors that, from an economic point of view, are very important.

### **2.3.1 Mechanisms of Drying**

Drying is a highly complicated process that remains poorly understood at the microscopic level due to challenges and limitations in accurately modeling it mathematically. According to Kudra and Mujumdar (2002) and Yilbas et al. (2003), It involves simultaneous and often coupled multiphase, heat, mass and momentum transfer phenomena.

The fundamental mechanism of moisture transfer is due to four major modes of transfer namely (Ibrahim Dincer & Calin Zamfirescu, 2016).

1. Capillary flow of moisture in small interstices.
2. Moisture diffusion due to concentration gradients.
3. Vapor diffusion due to partial pressure gradients.
4. Diffusion in liquid layers adsorbed at solid interfaces.

Generally, capillarity is mostly relaled to coarse granular materials, whereas liquid diffusion occurs in single-phase solids with colloidal or gel-like structure. In many cases, the two mechanisms may be applicable to a single drying operation, that is, capillarity dominating moisture movement in the early stages of drying, while taking over at lower moisture contents (Brennan et al., 1976).

### **2.3.2 Drying Phases**

During a drying process, the moisture content is usually calculated on a dry material basis. This indicates that the difference between the weights of the moist and dry materials yields the mass of moisture.The ratio between the mass of moisture (mm) and the mass of dry material (ms) represents the moisture ratio in percent on a dry basis; this is usually represented with the symbol MR or W. The variation of dry basis moisture ratio is usually measured versus the drying time and is called the moisture ratio history data (Ibrahim Dincer & Calin Zamfirescu, 2016). Moisture ratio typically ranges from 0 to 1.

The variation of moisture content during drying for a scenario in which a solid loses moisture is depicted in Figure 2.1a. When a solid is dried in hot air, the air serves as a carrier gas to remove the water vapor that forms around the evaporating surface and provides the moisture with the sensible and latent heat of evaporation that it needs. The process's initial phase, shown by curves A–B in Figure 2.1a, is caused by mass transfer from the solid surface. This is a stage of warming up of the solid(s) during which there is equilibrium between the surface of the solid and the drying air. In terms of consumption of energy, period A-B typically represents a very small percentage of the total energy required for the drying cycle, but in certain situations, this could be substantial (Ibrahim Dincer & Calin Zamfirescu, 2016).

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| **Figure 2.1**: The drying periods for a solid. (a) Moisture content versus time. (b) Drying rate versus drying time. (c) Drying rate versus moisture content. (The curves are for moist material dried at a constant temperature and relative humidity) (Ibrahim Dincer & Calin Zamfirescu, 2016). |

Depending on the prevailing conditions, the moist material may absorb more humidity during this period rather than drying out. The surface eventually reaches a point where the product's humidity diffuses out. The period A-B is governed mostly by transient heat transfer processes which can be diffusively or convectively controlled depending on the Biot number value.

The process B-C shows a reduction of the moisture content which is approximately linear with time. The saturated surface's area gradually shrinks throughout this period while the rate of water removal per unit of drying surface remains relatively constant. Point C, where the constant rate phase ends, is known as the point of critical moisture content. The solid's moisture moves quickly enough to maintain a saturated state at the surface during the B–C period, and the rate at which heat is transferred to the evaporating surface regulates the drying rate. Because the rate at which water moves from the solid to the surface is equal to the rate of evaporation, the solid's surface stays saturated with liquid water (or moisture). This stage is influenced by the area exposed to the drying medium, the heat and/or moisture transfer coefficients, and the temperature and relative humidity differences between the solid’s wet surface and the drying air (Ibrahim Dincer & Calin Zamfirescu, 2016).

The phase C–D, in which evaporation no longer occurs at the surface, comes after the saturated moisture at the surface has completely been removed. Rather, convective mass transfer at the solid's surface occurs after the moisture within the solid diffuses. The surface temperature starts to increase at point C and keeps increasing while drying goes on, getting closer to the air's dry-bulb temperature as the material gets drier. Consequently, the complete drying process takes place under conditions of constant rate when the initial moisture level is higher than the critical moisture content. If it is below the critical moisture content, the entire drying process occurs in the falling rate period solid (Ibrahim Dincer & Calin Zamfirescu, 2016).

Figure 2.1b illustrates how the drying rate varies with the solid's dry basis moisture content. The W(t) curve from Figure 2.1a is differentiated to get this curve. It should be noted that the drying rate remains constant during periods B–C, which is consistent with the linear decrease in moisture that is specific to the evaporative drying Furthermore, the rate at which moisture is removed decreases somewhat sharply with diffusive drying. Additionally, the drying rate vs drying time variation is displayed in Figure 2.1c.

Drying kinetics describes how a material’s average moisture content and temperature vary over time, whereas drying dynamics focuses on the variations in temperature and moisture distribution within the entire drying material. Drying kinetics is useful for calculating factors such as the amount of moisture evaporated, drying time, and energy consumption. These factors are significantly influenced by the physicochemical properties of the material. However, heat and moisture transport between the surface of the body, the environment, and the internal structure of the drying material typically controls changes in temperature and moisture content in the material. Factors such as temperature, humidity, air velocity, and total pressure significantly affects how the moisture content changes over time (Ibrahim Dincer & Calin Zamfirescu, 2016).

### **2.3.3 Heat Transfer in Dehydration**

#### **2.3.3.1 General Background**

The transfer of heat plays a major role in the dehydration of agro-products thus, its understanding is needed to improve control and avoid under or over-processing, which often results in negative effects on the product properties. There are two ways to transport heat to or from food: directly and indirectly. Direct methods allow contact between the food and the heating medium while indirect methods involve the use of heat exchangers that isolate the product from the medium used as a source or sink of heat (Sepúlveda & Barbosa-Cánovas, 2003).

A nonmechanical energy transfer between areas with varying temperatures is heat. In order to establish an equilibrium temperature, heat energy moves from a hotter point to a colder point, making heat transfer a natural energy transfer process. The physical condition of the bodies and their respective positions determine the heat transmission mode that controls the process. Conduction will be the method of heat transfer if there is a thermal gradient between two solid bodies in contact. Convection will transmit the energy if there is the same gradient between two fluids or between a fluid and a solid. Lastly, anybody with a temperature higher than absolute zero will emit energy in the form of electromagnetic waves transferring heat by radiation. In addition to the physical state or relative position, other physical properties of the materials involved in these processes play a crucial role in determining the heat transfer rate. Characteristics such as shape, size, structure, thermal conductivity, specific heat, density, and viscosity are vital in defining the behavior of a system (Sepúlveda & Barbosa-Cánovas, 2003).

#### **2.3.3.2 Heat Transfer by Conduction**

Heat transfer in solids or materials with high viscosity takes place by conduction (Sepúlveda & Barbosa-Cánovas, 2003). The flow of free electrons in metallic substances causes thermal conduction, therefore thermal conductivity and electrical conductivity are closely related. Thermal conduction occurs when individual molecules transfer momentum along a temperature gradient in most liquids and in solids that are poor electrical conductors. In gases, heat transfer by conduction occurs by the random movement of molecules, so that heat is “diffused” from positions of high temperature to positions of colder temperature (McCabe et al., 1993, pp. 286).

A body's internal temperature fluctuates over time as heat enters the body. The unsteady state period is the name given to this time frame. After heat transfer has occurred and equilibrium temperatures has been achieved, the internal temperature at each point in the body will remain constant with respect to time and will only only vary according to its relative location within the body. At this moment, The body is currently functioning as a heat conductor with a specified heat flux passing through it as the steady state transfer regime has been reached (Sepúlveda & Barbosa-Cánovas, 2003). Therefore heat transfer by conduction can be split into two main scopes; the study of heat conduction in the steady state and the study of heat conduction in the nonsteady state.

##### **2.3.3.2.1 Steady State**

Equation 2.1, the Fourier’s law for heat conduction which states that the heat flux Qx transmitted through a solid in the direction x is inversely proportional to the thickness x and directly proportional to the perpendicular transmission area A and the temperature difference between its two opposite faces ∆T can be used to model this mechanism. Thermal conductivity (K) is the proportionality constant required by this model.

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The negative sign depicts the temperature gradient i.e the flow of heat from a higher temperature to a lower temperature, thereby giving a positive value for the heat flux.

##### **2.3.3.2.2 Nonsteady State**

When studying operations that aim to heat or cool a body rather than use it as a heat conduction medium, the study of heat conduction in the nonsteady state becomes relevant. The aim is to determine the time it takes the hottest point in a body to reach the desired temperature (Sepúlveda & Barbosa-Cánovas, 2003).

Due to its restricted dimensions, heat transfer by conduction in agricultural goods is often a three-dimensional process. Mathematically the Fourier’s second law of heat transfer for three-dimensional nonsteady state heat conduction states that:

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Where T represents the temperature, t represents time, x, y, and z represents the distance on the x, y and z axis respectively, and α represents thermal diffusivity, which is a physical characteristic of the materials (Sepúlveda & Barbosa-Cánovas, 2003).

#### **2.3.3.3 Heat Transfer by Convection**

Convection is the process by which heat energy moves through a fluid due to the fluid's bulk movement caused by a temperature differential. The density variations cause the fluid molecules to move and interact with one another at various locations, exchanging energy (Sepúlveda & Barbosa-Cánovas, 2003). Most of the convectional heat transfer processing applications entail steady state transfer from a solid surface to a fluid that comes into contact with it, or the other way around. Convectional heat transfer can be represented by the Newton's law of cooling.

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Where Q represents the heat flux, A the interchange area, the difference between the fluid and solid temperatures, and h the proportionality coefficient, known as the heat transfer coefficient.

Temperature variations at various locations within the fluid might cause bulk molecular movement by creating a buoyant force. This process is known as natural convection. The coefficient of thermal expansion of a fluid (β) is the primary factor controlling natural convection. Natural convection would not be feasible in the absence of gravity and thermal expansion. In natural convection, the temperature gradient determines the mixing effectiveness. A small difference in temperature between the solid and fluid in contact will induce weak currents with a low heat transfer coefficient. However, regardless of natural convection, larger velocities and strong currents are produced when a fluid is forced to flow past a surface by mechanical means like a pump or fan. More effective mixing allows for the achievement of high heat transfer coefficients. Forced convection is the name given to this regime. In practical applications, forced convection is the most used convective heat transfer mode because it allows for higher heat transfer and better system control (Sepúlveda & Barbosa-Cánovas, 2003).

Newton’s law of cooling states that heat flux is directly proportional to the temperature gradient and contact area, both of which are readily quantifiable. However, figuring out the proportionality constant "h" presents a number of challenges. The density, viscosity, specific heat, and thermal conductivity of the fluid, the flow's properties (such as velocity, forced or natural convection, streamline or turbulent flow), and other system physical attributes like size and shape all affect this constant.

Researchers proposed a dimensionless expression that connects the heat transfer coefficient to particular characteristics of fluids and systems. This expression relates the Nusselt number Nu to the Reynolds (Re), Prandtl (Pr), and Grashof (Gr) numbers (Sepúlveda & Barbosa-Cánovas, 2003).

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A dimensionless representation of the heat transfer coefficient is the Nusselt number. The fluid's thermal conductivity (k) and the system's characteristic dimension (d), which is the diameter for a circular pipe or the length for a flat surface, are the other variables that affect this ratio.

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The Reynolds number provides details about the flow regime and fluid properties. It relates macroscopic flow to internal friction. The inertial force takes over and changes the flow from a laminar to a turbulent state when this ratio rises above a particular threshold. This number relates the fluid’s density (ρ), viscosity (η), velocity (v), as well as the characteristic dimension (d) (Sepúlveda & Barbosa-Cánovas, 2003).

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The Prandtl ratio behaves as a physical constant and addresses the fluid’s physical characteristics. This expression involves thermal conductivity (k), specific heat (Cp) and viscosity (η).

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Lastly, the ratio of buoyancy to internal friction is represented by the Grashof number. This number shows the relationship between the characteristic size of a body (d), the acceleration caused by gravity (g), the thermal expansion coefficient β, fluid’s density (ρ), its viscosity (η), and the temperature difference between a surface and the fluid ∆T:

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#### **2.3.3.4 Heat Transfer by Radiation**

Another mode of heat transfer is by radiation. A body with a temperature higher than absolute zero will emit electromagnetic radiation. The wavelength decreases as the temperature rises because the radiation becomes more energetic. Radiation heat transfer happens continuously throughout nature since it doesn't need a temperature gradient to occur.

Any given mass of material will emit radiation regardless of whether another material is in close proximity to or in contact with the material. The difference between the energy a body generates and the energy it absorbs from radiation released by other bodies is known as its net energy gain or loss.

When two bodies with a temperature difference are placed in sight of one another inside an enclosure, the hotter body loses heat through radiation emission more quickly than it gains from radiation absorption from the cooler counterpart, causing the temperature of the hotter body to decrease. At the same time, the cooler body absorbs heat from the hotter ones faster than it emits heat, causing its temperature to increase. Similar to heat transfer by conduction and convection, equilibrium is attained when all of the bodies reaches the same temperature. The common practice of referring to radiation as "heat" is justified by the fact that it is converted into heat upon absorption and that temperature equilibrium is reached through the net transfer of radiation (McCabe et al., 1993, pp. 398).

The heat flux density exchanged between two parallel plates at temperatures Ts and Ta is given by

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Where  is called the emissivity, is the Stefan-Boltzmann constant, having a value of W/m2K4 while Ts represents the absolute temperature of the surface

### **2.3.4 Mass Transfer in Dehydration**

Mass transfer is the movement of chemical species from one location to another. During drying, the concentration gradients cause moisture to move from different cellular sites to the material's surface. Then, the surface moisture moves to the environment (drying air) by evaporation (Khan et al., 2018). The first process can be defined as an internal mass transport process where moisture moves from one location to another inside the material while the second process can be defined as an external mass transport process in which the moisture moves from the surface of the material to the drying air inside the dryer (Khan et al., 2022).

The major driving forces of internal and external transport process are Diffusion, Convection and Evaporation (Khan et al., 2022).

#### **2.3.4.1 Diffusion**

Diffusion is a process of molecular mass transfer in which molecules are randomly transferred from regions of high concentration to low concentration areas; no molecules have a favoured direction in this process. Moisture moves through a medium using two distinct diffusion processes: capillary diffusion and binary diffusion.

Capillary diffusion: The Capillary action of the liquid is the main force behind the mass transfer process known as capillary diffusion. The capillary action is created by capillary forces which are the molecular attraction between the liquid molecules and the solid surfaces (Khan et al., 2022). The capillary actions are increased by the interfacial pressure differential within the porous matrix.

The capillary flow in a porous media can be expressed by Darcy’s law (Datta, 2007):

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Where P represents the pressure of the fluid (Pa), u represents the Darcy velocity (m/s), kl represents the porous material’s permeability (m2), and µ represents the dynamic viscosity (Pa.s).

Sometimes, the capillary action is expressed as a function of negative pressure on the liquid (Datta, 2007). Therefore, the mass transfer (mass flux) of the liquid can be expressed by:

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|  | 2.11 |

Where represents the mass flux of the liquid due to the capillary effects (kg/m2s), and µl represents the density (kg/m3) and the dynamic viscosity of the liquid (Pa.s) respectively. P indicates the total gas pressure (Pa), pc represents the liquid phase capillary pressure, and s the distance (m).

Binary Diffusion: This is a process of gaseous species (air and vapor) mass transfer. The binary diffusion coefficient plays a significant role in expressing the gas species movement from one medium to another. Fuller et al (1966) mathematically expressed the binary coefficient (DAW) of species A to diffuse through a medium W using the following equation.

|  |  |
| --- | --- |
| DAW = | 2.12 |

Where MA and Mw are the air and water species molecular weight (g/mol) respectively. P is the external pressure (atm), and represents the vapour and air atomic diffusion volume, respectively, and Tf represents the average temperature between the environment temperature and the material surface temperature (K).

The Bolz formula can also be used to express binary diffusion coefficients as a function of temperature, as:

|  |  |
| --- | --- |
| DAW = | 2.13 |

Where T represents the temperature (K).

#### **2.3.4.2 Convection**

Convection is one of the main mass transfer mechanisms that occurs in fluid motion. The pressure-driven flow is one way to depict mass transfer caused by convection. Moisture migrates from a region of higher-pressure to a region of lower-pressure when a pressure gradient is present in a multiphase porous domain, like food ingredients (Khan et al., 2022). When it comes to heating in an enclosed case, such microwave-based heating or frying, pressure-driven flow is crucial.

**2.3.4.3 Evaporation**

Evaporation is the process by which heat energy is absorbed and a liquid changes phase into a vapor. In a porous media, evaporation can happen in three different ways, according to Khan et al. (2022):

1. Distributed (equilibrium) evaporation
2. Non-equilibrium evaporation.
3. Evaporation in the moving interface at the boundary.

The non-equilibrium evaporation rate () can be calculated by the following equation

|  |  |
| --- | --- |
|  | 2.14 |

Where the molecular weight of vapour (kg/mol) is represented by Mv, the vapour pressure (Pa) is represented by Pv, the gas constant (kg/mol/K) is represented by R, the evaporation constant (1/s) represented by Kc, and the equilibrium vapour pressure (Pa) which is represented by Pv,eq .

According to Mercier et al. (2014), the evaporation caused by the difference in density between the equilibrium vapour density ) and the actual vapour density () is directly proportional to the non-equilibrium evaporation and is expressed as follows.

|  |  |
| --- | --- |
|  | 2.15 |

Where Kp represents the proportionality constant.

## 2.4 Mathematical Modelling of Drying

Mathematical modeling of drying provides a structured approach to describe and predict the behavior of moisture and heat within a material during the drying process. These models serve several purposes, such as aiding in the design of drying equipment, optimizing operating conditions, reducing energy consumption, and improving product quality (Turan & Fıratlıgil, 2019). They also enable researchers and engineers to simulate drying under different scenarios without the need for exhaustive experimental trials, saving time and resources.

Drying processes are modeled with two main models:

1. **Distributed models**

Simultaneous mass and heat transfer are taken into account in distributed models. They more accurately forecast the product's temperature and moisture gradient by accounting for both internal and exterior heat and mass transfer (Erbay & Icier, 2010).

1. **Lumped parameter models**

The product's temperature gradient is not taken into account by lumped parameter models. They make the assumption that the product's drying air temperature is equal to a uniform temperature distribution (Erbay & Icier, 2010). By decreasing the product's thickness, this assumption can be brought down to acceptable levels and only leads to inaccuracies at the start of the drying process (Henderson & Pabis, 1961).

### **2.4.1 Thin Layer Drying Models**

According to the American Natl. Standards Inst. And the American Society of Assoc. Executives (ANSI/ASAE 2014), a thin-layer is a layer of material fully exposed to an airstream during drying. The thickness of the layer should be uniform and should not exceed 6mm (Onwude et al., 2016). Because of its thin structure, a uniform temperature is assumed and thus, is very suitable for lumped parameter models (Erbay & Icier, 2010).

Thin layer drying models have been found to have wide applications due to their easy usage and requirement of less data (Madamba et al., 1996; Ozdemir & Devres, 1999). According to Onwude et al (2016), It is important to note that the concept of thin-layer drying can be applied to:

1. One layer of the material freely exposed to the drying air.
2. A multilayer of different slice thickness, so far the relative humidity of the drying air and the drying temperature remain in the same thermodynamic state throughout the drying process.

Thin layer models can be theoretical, semi-theoretical or empirical.

Theoretical models consider both the external and internal resistance to moisture transfer. According to Onwude et al. (2016), these includes the material's conductivity, mass diffusivity, and shape. Although theoretical models are applicable to all process settings and provide a clear explanation of the product's drying characteristics, they contain numerous assumptions that lead to significant mistakes (Erbay & Icier, 2010). The most commonly used theoretical models are derived from the Fick’s second law of diffusion.

Semi-theoretical models are derived from the theoretical model (Fick’s second law of diffusion) or its simplified version (Newton’s law of cooling). These models assume that the the product's exterior layer is where the resistance to water diffusion takes place (Ertekin & Firat, 2015). Because semi-theoretical models make use of some experimental data, they are simpler and require fewer assumptions. However, they are only applicable within the parameters of the drying process such as the drying temperature and thickness of the material being dried (Fortes & Okos, 1981; Parry, 1985).

Empirical models gives a direct relationship between the average moisture content and the drying time. The primary drawback of using empirical models in thin-layer drying is that they provide erroneous parameter values because they do not have any theoretical background, and are solely derived from experimental data (Onwude et al., 2016).

#### **2.4.1.1 Models Derived from Newton’s Law of Cooling**

1. **Newton model:** The newton’s model also known as the exponential model is the simplest model because it has only one model constant ‘k’. researchers have used this model to describe the drying behavior of several agro-products (Onwude et al., 2016).

|  |  |
| --- | --- |
|  | 2.16 |

where k is the drying constant (s-1), MR is the moisture ratio, M is the dry basis moisture content at any time t, MO is the initial dry basis moisture content of the sample, and Me is the equilibrium moisture content. Additionally, the drying behaviour of red chiles and strawberries has been found to be adequately described by the Newton model. (Onwude et al., 2016).

1. **Page model:** The page model or the Modified Lewis model is a modification of the Newton’s model. The errors associated with the Newton’s model are greatly minimized by the addition of a dimensionless empirical constant (n).

|  |  |
| --- | --- |
|  | 2.17 |

Where n is the model constant (dimensionless).

This model is widely used as the basis for most semi-theoretical thin-layer models. Doymaz (2007a) predicted the drying characteristics of tomato using this model. Rafiee et al (2008) also used the Page’s model to predict the drying characteristics of wheat.

1. **Modified Page Model:** This is a modification of the page model.

|  |  |
| --- | --- |
|  | 2.18 |

Equation 2.18 is widely regarded as the Modified Page model (II). This model has 2 constants and has been applied in predicting the drying kinetics of mint leaves (Onwude et al., 2016).

1. **Otsura et al. Model:** Ertekin and Firat (2015) used the Otsura et al. model for the thin layer drying modelling of rough rice.

|  |  |
| --- | --- |
|  | 2.19 |

#### **Models Derived from Fick’s Second Law of Diffusion**

1. **Simplified Fick’s Model**

Kumar et al (2006) described the simplified solution of Fick’s diffusion equation valid for long drying times by

|  |  |
| --- | --- |
|  | 2.20 |

Togrul and Pehlivan (2002) used this equation to model the drying of apricot while Gunhan et al (2005) used it to model the drying of bay leaves.

1. **Henderson and Pabis model:**

This model is also known as the single-term model. It is the first term of the general solution of the Fick’s second law of diffusion. The Henderson and Pabis (1961) model has been effectively applied in the drying of crops such as corn and millet (Onwude et al., 2016).

|  |  |
| --- | --- |
|  | 2.21 |

Where a represents the shape of the material used (dimensionless).

This model effectively predicts the drying rate at the beginning of the drying process, but appears sometimes to be less efficient for the last stages of the process (Dissa et al., 2008).

1. **Modified Henderson and Pabis model:**

The modified Henderson and Pabis model is a third term general solution of the Fick’s law of diffusion for correction of the shortcomings of the Henderson and Pabis model. It has been reported that the first term explains the falling rate period in the drying process of agro-products (Onwude et al., 2016). This model contains six constants and thus, can be regarded as a complex thin-layer model.

|  |  |
| --- | --- |
|  | 2.22 |

Where a, b and c are dimensionless model constants and k, g and h are drying constants (s-1).

1. **Logarithmic (Asymptotic) model:**

Chandra and Singh (1995) proposed this model which is the Henderson and Pabis model written in logarithmic with the addition of an empirical term ‘c’.

|  |  |
| --- | --- |
|  | 2.23 |

Where c is a dimensionless constant.

1. **Two-term model:**

This model is the first two terms of the general series solution of the Fick’s second law of diffusion. The model contains 2 dimensionless empirical constants and 2 model constants which can be derived from experimental data. The two-term model assumes a uniform product temperature and diffusivity throughout the drying period. Hence, it can be used to model the drying process of materials with high moisture content such as fruits and vegetables (Onwude et al., 2016).

|  |  |
| --- | --- |
|  | 2.24 |

Where a and b are the dimensionless empirical constants, and K1 and K2 are the drying constants (s-1).

1. **Midilli et al model**:

A new model was proposed by Midilli et al. (2002) that was similar to the Henderson and Pabis model with the addition of a linear term. They applied this new model to the drying of mushroom and pollen using different drying methods.

|  |  |
| --- | --- |
|  | 2.25 |

1. **Demir et al. model:**

This model modifies both the Henderson and Pabis model and the Logarithmic model. It was proposed by Demir et al. (2007) for drying of green olives. It contains 4 constants and 3 dimensionless empirical constants.

|  |  |
| --- | --- |
|  | 2.26 |

1. **Verma et al. model:**

This model is a modification of the two-term model with 4 model constants. The Verma et. al (1985) model has been used successfully to describe the drying kinetics of parsley and pumpkin.

|  |  |
| --- | --- |
|  | 2.27 |

#### **Empirical models**

Empirical models give a direct relationship between the average moisture content and the drying time. The primary drawback of using empirical models in thin-layer drying is that they provide erroneous parameter values because they do not adhere to the theoretical fundamentals of the drying process, which takes the form of a kinetic relationship between the rate constant and the moisture concentration. Furthermore, these models do not have a physical interpretation and are entirely derived from experimental data (Onwude et al., 2016).

The 3 most widely applied empirical models for the dehydration of agro products are the

1. Weibull model.
2. Wang and Singh model.
3. Thompson model.
4. Diamante et al. model.
5. **Aghbashlo et al. model**:

Aghbashlo et al (2009) proposed a model that effectively described the thin-layer drying kinetics of biological materials. This model well describes the drying behaviour of carrots (Onwude et al., 2016). Just like other empirical models, there is no theoretical background for this model.

|  |  |
| --- | --- |
|  | 2.28 |

Where K1 and K2 are drying constants.

1. **Wang and Singh model:**

Wang and Singh (1978) developed this model to describe the drying behaviour of rough rice.

|  |  |
| --- | --- |
|  | 2.29 |

Where ‘a’ and ‘b’ are dimensionless constants gotten from experimental data.

1. **Diamante et al model:**

Diamante et al (2010b) proposed an empirical model for the drying of fruits and just like other empirical models, this model lacks theoretical background.

|  |  |
| --- | --- |
|  | 2.30 |

Where ‘a’, ‘b’, and ‘c’ are model constants.

1. **Thompson model:**

This model is an empirical model obtained from experimental data by correlating the drying time as a function of the logarithm of the moisture ratio. Pardeshi et al (2009) used this model to describe the drying kinetics of green peas.

|  |  |
| --- | --- |
|  | 2.31 |

1. **Weibull Distribution model:**

This model has no physical meaning. It is a pure statistical approach and given as the following equation (Ertekin & Firat, 2015). It has no physical meaning or a theoretical background. It is solely derived from experimental data.

|  |  |
| --- | --- |
|  | 2.32 |

## Parameters Estimation during drying

### **Estimation of effective moisture diffusivity during drying**

The effective moisture diffusivity is a function of temperature and moisture content of a material. It is a very crucial transport parameter used in the modelling of the drying process of fruits and vegetables (Onwude et al., 2016). It is estimated from the modified Ficks second law of diffusion using a slab geometry as:

|  |  |
| --- | --- |
|  | 2.33 |

Equation 2.33 can be linearized and expressed in a logarithmic form as:

|  |  |
| --- | --- |
|  | 2.34 |

Where:

Deff represents the effective moisture diffusivity (m2/s).

L represents the half thickness of the species (m).

t represents the time (secs).

MR represents the moisture ratio (dimensionless).

### **Estimation of the activation energy**

It is assumed that an Arrhenius function governs the relationship between effective moisture diffusivity and temperature (Onwude et al., 2016; Pardeshi et al., 2009). It is expressed mathematically as:

|  |  |
| --- | --- |
|  | 2.35 |
|  |  |

Equation 2.35 can be linearized and expressed in a logarithmic form as:

|  |  |
| --- | --- |
|  | 2.36 |

Where:

Deff is the effective moisture diffusivity (m2/s).

DO is the moisture diffusivity when time = 0.

T represents the temperature (K).

Ea represents the activation energy (kJ/mol).

R represents the universal gas constant (8.314 J/mol K)

## Data Analysis

Data analysis is a systematic process of inspecting, organizing, transforming, and modeling data with the objective of discovering useful information, drawing conclusions, and supporting decision-making. It is a fundamental component of research and scientific inquiry enabling individuals to make data-driven decisions based on empirical evidence.

Data analysis involves breaking down complex datasets into manageable parts, identifying patterns, trends, relationships, anomalies, and interpreting them to generate meaningful insights. Data analysis can be broadly classified into two types namely Quantitative data analysis and Qualitative data analysis.

### **Quantitative Data Analysis**

Quantitative data analysis is an organized method of evaluating numerical data. It involves the use of statistical methods, mathematical models, and computational techniques to identify patterns, relationships, and trends within a dataset.

#### **2.6.1.1 Methods of Quantitative Data Analysis**

In general, quantitative data analysis uses two methods to extract valuable insights from datasets. Descriptive statistics, the first approach highlights and illustrates key characteristics of a dataset, including the mean, median, and standard deviation.

The second approach known as inferential statistics, uses regression analysis and hypothesis testing to extrapolate conclusions and predictions from a sample dataset.

##### **2.6.1.1.1 Descriptive Statistics**

As the name suggests, descriptive statistics is used to describe a dataset; it is used to understand the specifics of the data by summarizing it and identifying patterns from the particular data sample; it is primarily used for analysing single variables and provides absolute numbers without necessarily providing an explanation for the numbers. It is often the first step in data analysis, laying the foundation for more advanced techniques like diagnostic or predictive analysis.

**Techniques used in Descriptive statistics**

1. **Measures of Central Tendency:**
2. Mean: This is a set of values numerical average. It is calculated by dividing the total number of observations by the sum of all values.
3. Median: This is used to get the midpoint of a set of values when the numbers are arranged in numerical order.
4. Mode: This is the most frequently occurring value in a dataset.
5. **Measures of Dispersion:**
6. Range: This is the difference between the highest and lowest values in a dataset.
7. Variance: This measures how much the data points differ from the mean.
8. Standard Deviation: This is an indication of how much individual data points deviate from the mean, giving a sense of data spread.
9. **Percentage:** This is used to show the relationship between a subset of respondents within a data and a larger group of respondents.
10. **Skewness:** This is a measure of the deviation of a random variable’s given distribution from the normal distribution.

##### **2.6.1.1.2 Inferential Statistics**

The goal of quantitative analysis is to use numerical values to transform raw data into meaningful insight. Descriptive statistics focuses on using numbers to explain the specifics of a given dataset, but they are unable to explain the motives behind the numbers, necessitating additional analysis using inferential statistics (Eteng, 2022).

The goal of inferential statistics is to make predictions or highlight possible outcomes from the data. They are used to generalize results, make predictions between groups and show relationships that exist between multiple variables.

Some of the statistical methods used within inferential statistics includes:

1. **Correlation Analysis:** Correlation analysis is a statistical method used to measure the strength of the linear relationship between two variables. It helps to identify how two things might be connected and how string that connection is (QuestionPro, 2024).
2. **Cross Tabulation:** This is a table used in statistics to display the relationship between two or more categorical variables. It allows to examine how different categories or group of variables intersect and how they are distributed within a dataset (Bock, 2018).
3. **Time Series Analysis**: Using statistical analysis, this method finds patterns and cycles across time. In order to identify trends, seasonality, and cyclic patterns, the same variables are measured at various points in time (Eteng, 2022).
4. **Cluster Analysis:** Cluster analysis is a technique used to group similar data points based on certain characteristics. It helps to identify patterns in data without predefined categories.
5. **Analysis of variance (ANOVA):** This is a statistical analysis done to assess the significance of how the average of two or more groups differ from each other (Eteng, 2022).
6. **Regression Analysis**

#### **2.6.1.2 Regression Analysis**

Regression Analysis is a statistical method used to examine the relationship between a dependent variable and one or more independent variables, with the primary aim of predicting the value of the dependent variable based on the known values of the independent variables.

According to Sarstedt and Mooi (2014), the key benefits of using regression analysis are that it can:

1. Show the significance of the relationship between an independent variable and a dependent variable.
2. Show the effects of the relative strength of the independent variables on the dependent variable.
3. Forecast the value of the dependent variable.

#### **2.6.1.3 The Basic Types of Regression**

The most common forms of regression analysis are:

1. **Simple Linear Regression**

Simple linear regression uses one independent variable (x) to explain or predict the outcome of the dependent variable (y). For example, Massie and Rose (1997) applied a simple linear regression methos to predict daily maximum temperatures investigated at Nashville, Tennessee.

The simple linear regression model is expressed using the following equation:

|  |  |
| --- | --- |
|  | 2.37 |

Where: y = variable predicted (dependent variable),

x = variable being used to predict (independent variable).

c = the intercept.

m = the slope.

1. **Multiple Linear Regression**

This is similar to the simple linear regression except that multiple independent variables (x1, x2, x3) are used in the model. Multiple linear regression is expressed mathematically as:

|  |  |
| --- | --- |
|  | 2.38 |

Where:

y = variable predicted (dependent variable),

x1, x2, x3 = variables being used to predict (independent variables).

b, c, d = model constants.

For example, Paras and Mathur (2012) used multiple linear regression to develop a model for forecasting weather parameters. Their study revealed that the proposed model could effectively predict weather conditions for a specific location using locally gathered data.

Multiple linear regression follows the same conditions as the simple linear regression, however, due to the presence of several independent variables in multiple linear regression, it is required that no collinearity exists between the independent variables.

1. **Non-Linear Regression**

Nonlinear regression is a type of regression analysis where data is fitted to a model and represented as a mathematical equation. Simple linear regression relates two variables (X and Y) with a straight line (y = mx + b), while nonlinear regression relates the two variables in a nonlinear (curved) relationship.

Non-linear regression modeling is similar to linear regression modeling in that both seek to track a particular response from a set of variables graphically. Nonlinear models are more complex to develop compared to linear models as their functions are created through a series of approximations (iterations), often involving trial-and-error.

To achieve these approximations, mathematicians utilize well-established techniques such as the Gauss-Newton method and the Levenberg-Marquardt method (Osorio, 2025). Moisture ratio history data are usually fitted to thin layer drying models using Nonlinear regression.

#### **2.6.1.4 Statistical Methods for Determination of Appropriate Models in Regression Analysis**

Some of the statistical methods used to determine the best model in regression analysis includes:

1. **Coefficient of determination (R2):** is a statistical measure that indicates how well a regression model explains the variability of the dependent variable. It is commonly used to assess the goodness of fit of a model. It ranges between 0 and 1. The closer it is to 1, the greater relationship exists between the experimental and predicted value (Ertekin & Firat, 2015).

|  |  |
| --- | --- |
|  | 2.39 |

Where:

is the predicted value.

is the observed value

is the mean of the observed value

n is the number of observations.

1. **Root-mean-square error (RMSE):** The root-mean-square error (RMSE) is a commonly used metric to quantify the discrepancies between the values that are actually seen from the process being modelled or estimated and the values that are by predicted by the model. RMSE is a good measure of accuracy and serves to combine the residuals into a single measure of predictive power. It is required to reach zero (Ertekin & Firat, 2015). It can be mathematically expressed by:

|  |  |
| --- | --- |
|  | 2.40 |

Where:

is the predicted value.

is the observed value.

n is the number of observations.

1. **Sum of squares error (SSE):** this is the difference between the observed and forecasted values. It can be mathematically represented by:

|  |  |
| --- | --- |
|  | 2.41 |

Where is the difference between the actual value of the dependent variable and the predicted value. Regression analysis aims to minimize the SSE. The smaller the SSE, the better the model’s estimation power.

### **Qualitative Data Analysis**

Qualitative analysis is a branch of data analysis that interpretes non-numeric data to uncover patterns, themes, and insights. It is commonly applied in disciplines such as social sciences, education, and healthcare. Unlike quantitative analysis, which relies on numerical data and statistical techniques, qualitative analysis explores the underlying meaning of data, offering context and a deeper understanding that numerical values alone cannot provide. (Stewart, 2024).

# CHAPTER THREE: METHODS AND MATERIALS

## Introduction

This chapter covers information on the materials, tools and methods used to develop and validate the computer software for analyzing data from agro-products dehydration. The software is designed to perform the following tasks:

1. Allow users to upload an excel file containing moisture ratio history data.
2. Calculation of moisture diffusivity from the uploaded data.
3. Calculation of thermodynamic properties which includes the activation energy, enthalpy, entropy and Gibbs free energy.
4. Fitting of the moisture ratio history data to multiple thin-layer drying models using non-linear regression.
5. Evaluation of performance metric of models using statistical parameters (R2, RMSE, & SSE).
6. Determination of the best model based on the performance metric
7. Prediction of moisture ratio using model.
8. Data generation for drying, drying rate and Krischer plots.
9. Creation of the drying, drying rate and Krisher plots.

The procedures followed in the software development, data collection, and results validation are outlined in this chapter.

## Materials

The materials used for this research include both hardware and software tools necessary for software development and data analysis.

### **Hardware**

The following hardware components were used:

1. A personal computer with the following specifications:

* Processor: Intel(R) Core(TM) i5-8350U CPU @ 1.70GHz 1.90 GHz.
* Installed RAM: 8.00 GB.
* Storage Capacity: 256GB SSD.

### **Software and Programming Tools**

The software was developed using the following programming tools:

1. Programming Language: Python (Version 3.13.0)
2. Python Packages.

|  |  |  |
| --- | --- | --- |
| **Table 3.1: Packages and their respective versions** | | |
| **S/N** | **LIBRARY** | **VERSION NO** |
| 1 | altgraph | 0.17.4 |
| 2 | colorama | 0.4.6 |
| 3 | contourpy | 1.3.1 |
| 4 | control | 0.10.1 |
| 5 | CTkMenuBar | 0.8 |
| 6 | customtkinter | 5.2.2 |
| 7 | cx\_Freeze | 7.2.7 |
| 8 | cx\_Logging | 3.2.1 |
| 9 | cycler | 0.12.1 |
| 10 | darkdetect | 0.8.0 |
| 11 | decorator | 5.2.1 |
| 12 | et\_xmlfile | 2.0.0 |
| 13 | Fonttools | 4.55.3 |
| 14 | Imageio | 2.37.0 |
| 15 | imageio-ffmpeg | 0.6.0 |
| 16 | joblib | 1.4.2 |
| 17 | kiwisolver | 1.4.7 |
| 18 | lief | 0.15.1 |
| 19 | markdown-it-py | 3.0.0 |
| 20 | matplotlib | 3.10.0 |
| **S/N** | **LIBRARY** | **VERSION NO** |
| 21 | mdurl | 0.1.2 |
| 22 | moviepy | 2.2.1 |
| 23 | mpmath | 1.3.0 |
| 24 | Nuitka | 2.5.7 |
| 25 | numpy | 2.1.3 |
| 26 | openpyxl | 3.1.5 |
| 27 | ordered-set | 4.1.0 |
| 28 | packaging | 24.2 |
| 29 | pandas | 2.2.3 |
| 30 | pefile | 2023.2.7 |
| 31 | pillow | 11.0.0 |
| 32 | proglog | 0.1.12 |
| 33 | Pygments | 2.19.1 |
| 34 | pyinstaller | 6.11.1 |
| 35 | pyinstaller-hooks-contrib | 2024.10 |
| 36 | pyparsing | 3.2.0 |
| 37 | python-dateutil | 2.9.0.post0 |
| 38 | python-dotenv | 1.1.0 |
| 39 | pytz | 2024.2 |
| 40 | pywin32-ctypes | 0.2.3 |
| 41 | rich | 13.9.4 |
| 42 | scikit-learn | 1.6.0 |
| 43 | scipy | 1.14.1 |
| 44 | setuptools | 75.6.0 |
| 45 | six | 1.17.0 |
| 46 | sympy | 1.13.3 |
| 47 | threadpoolctl | 3.5.0 |
| **S/N** | **LIBRARY** | **VERSION NO** |
| 48 | tqdm | 4.67.1 |
| 49 | tzdata | 2024.2 |
| 50 | XlsxWriter | 3.2.2 |
| 51 | zstandard | 0.23.0 |

1. Version control and documentation: GitHub (www.github.com)

## Software Architecture and Design

The software is built on a modular architecture that segregates data reading, data writing computational modeling and the user interface.

1. Data Reader Module: This module is responsible for handling file imports and reading. It contains functions that accepts moisture ratio history data from users in ‘.xlsx’ (excel) format and extracts all the necessary parameters such as temperature, thickness of species, time, and MR variations.
2. Data Writer Module: This module handles all data writing to file tasks such as report generation for models fitting, result generation for moisture diffusivity calculation, result generation for all thermodynamic parameter calculations which includes Enthalpy, Entropy and Gibbs free energy.
3. Model Fitter Package: This package contains several modules which are responsible for fitting the moisture history data several thin layer drying models through non-linear regression. The modules contain a function that performs a maximum of 50,000 iterations for each model using the Levenberg-Marquardt or the Trust Region Reflective algorithm to estimate the model constants.
4. The package also contains modules that evaluates the performance of each model by calculating the coefficient of determination (R2), Root mean square error (RMSE), and the sum of square error (SSE).
5. Thermodynamics Package: This package contains a module that performs all the thermodynamic calculations. The functions in the module carries out the respective linear regressions required for the calculation of the moisture diffusivity, activation energy, enthalpy, entropy and Gibbs free energy.
6. The main module: This module is responsible for bringing all the different parts of the software together, it incorporates all the functions defined in all the other modules and packages, ensuring efficient file reading, data extraction, models fitting and reports generation.
7. User interface: An intuitive graphical user interface that allows end users to input data and get analysis results built with Tkinter and CustomTkinter.

## Implementation of Data Analysis Algorithms

The core functionality of the software involves integration of algorithms for model fitting and data analysis.

1. **Regression and Model Fitting:** Utilizes the SciPy and scikit-learn libraries to perform both linear and Nonlinear regression for fitting experimental data to various equations.
2. **Error and Performance Metrics:** Computes statistical metrics including the coefficient of determination (R2), Root Mean Square Error (RMSE) and the Sum of Squared Error (SSE) to access model accuracy.
3. **Optimization Techniques:** Utilizes iterative algorithms such as the Levenberg-Marquardt and the Trust Region Reflective algorithms to refine model parameters and enhance fit.

## User interface and Usability Testing

1. **Data import/Export Functionality:** Users can easily upload datasets contained in several sheet in a single excel file. The results of the analysis are automatically exported and saved on the user’s computer.
2. **Usability Testing:** The interface will be evaluated by a sample of potential end-users whose feedback will be used to enhance the software’s usability and functionality.

## Error Handling

Error handling was implemented to ensure smooth operation and user-friendly interaction. The aim was to anticipate possible issues that may arise during file selection, data loading, model fitting and provide useful feedback rather than allowing the software to crash unexpectedly. A help menu bar containing the documentation was also created to guide the users on how to use the software.

### **Possible causes of error**

1. Missing or inaccessible uploaded file.
2. Incorrect file structure.
3. Incorrect data format.
4. Incorrect data type.
5. Model convergence failure.

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| **Figure 3.1**: Code snippet of error Handling |

## Software Naming and Versioning

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| **Figure 3.2**: Flowchart Describing the Drying Software Operation. |