DEVELOPMENT OF HEAT AND MASS TRANSFER CONSTITUTIVE MODEL FOR PARCHMENT COFFEE DEHYDRATION PROCESS

By

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Abstract

This thesis presents a mathematical constitutive model, based on the volume averaging method, to predict the temperature and wet based moisture content of parchment coffee during the dehydration process using rotary drum technology. The model considers the two main stages of the dehydration process: 1) the funicular stage which is characterized by the vaporization of water, and 2) the pendular stage which is dominated by convective diffusive phenomena. These driving forces depend on the topological characteristics of the studied porous medium. Mathematical estimates of parameters such as the permeability were performed due to lack of published data. Numerical results are obtained using the finite volume method and appropriate discretization schemes. To validate the model, data from a scale rotary drum dryer was used. The error of the predicted values is characterized by a percentage difference of $9.14\% \pm 7.69\%$ for temperature and $14.17\% \pm 9.13\%$ for wet-base moisture content.

Resumen

Esta tésis presenta un modelo matemático constitutivo, basado en el método de volumen promediado, para predecir la temperatura y el contenido de humedad de la masa de café pergamino durante el proceso de deshidratación utilizando la tecnología de batea. El modelo considera las dos etapas principales de este proceso: 1) la etapa funicular, caracterizada por la evaporación de agua, y 2) la etapa pendular, dominada por fenómenos de convección y difusión. Estos fenómenos dependen de la topología del medio poroso estudiado. Se realizaron estimados matemáticos de parámetros como la permeabilidad debido a la falta de datos publicados. Los resultados numéricos se obtienen utilizando el método de volumen finito y esquemas apropiados de discretización. Para validación del modelo, se utilizaron los datos de un secador tipo batea a escala. El error de estas predicciones es caracterizado por un porciento de diferencia de 9.14% \pm 7.69% para temperatura y 14.17% \pm 9.13% para el contenido de humedad.

Declaration of Authorship

I, Moises Ocasio, declare that this thesis titled, "DEVELOPMENT OF HEAT AND MASS TRANSFER CONSTITUTIVE MODEL FOR PARCHMENT COFFEE DEHYDRATION PROCESS" and the work presented in it are my own. I confirm that:

- 1 This work was done wholly or mainly while in candidature for a research degree at this University.
- 2 Where any part of this thesis has previously been submitted for a degree or any other qualification at this University or any other institution, this has been clearly stated.
- **3** Where I have consulted the published work of others, this is always clearly attributed.
- 4 Where I have quoted from the work of others, the source is always given. With the exception of such quotations, this thesis is entirely my own work.
- 5 I have acknowledged all main sources of help.
- 6 Where the thesis is based on work done by myself jointly with others, I have made clear exactly what was done by others and what I have contributed myself.

Signature

Date

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List of Symbols

Roman symbols

Cross-sectional area of flow (m ²	A
Surface area of β - γ interface (m ²	$A_{\beta\gamma}$
Moisture diffusivity (m ² /s)	a_m
Concentration (kg-m ⁻³	С
Capillary numbe	Ca
Specific heat (J/kg-K	С
Mass fraction weighted specific heat (J/kg-K	c_p
Phase average specific heat (J/kg-K	$\langle c_p \rangle^i$
Diffusion conductance at cell face (W/m ² -K	D
Diffusivity Coefficient (m ² /s	D
Capillarity mass transfer coefficien	D'
Diffusion mass transfer coefficien	D''
Mean equivalent diameter (m	D_e
Percentage difference	6diff
Effective diffusivity coefficient (m ² /s	$D_{e\!f\!f}$
Total energy (J	Ε
Convective mass flux per unit area (kg/m ² -s	F
Fourier numbe	Fo
Gravitational acceleration of the earth (m/s ²	g
Gravity potential vector (m/s ²	ţ
Gravity numbe	Gr
Specific enthalpy (J/kg	Н
Latent heat of vaporization (J/kg	h_{vap}
Mass flux (kg/s-m ²	J
Permeability of the medium (m ²	Κ

$k_{e\!f\!f}$	Effective thermal conductivity (W/m-K)
K_i	Permeability of the ith species (m ²)
<i>k</i> _{<i>i</i>}	Phase thermal conductivity (W/m-K)
k _c	Capillary pressure mass coefficient
$k_{\langle T angle}$	Capillary pressure temperature coefficient
L	Characteristic length of the flow (m)
î	Dimensionless length
l _c	Critical length
M	Number of liquid phase discontinuities
m_i	Mass of ith species (kg)
$\langle \dot{m} angle$	Vaporization rate (kg/m ³ -s)
MR	Moisture rate
п	Number of pore sizes
Р	Pressure (Pa)
P_{c}	Capillary Pressure (Pa)
Pe	Peclet number
P_{i}	Total pressure of ith species (Pa)
P_{0}	Reference pressure (Pa)
Pr	Prandtl number
P _{sat}	Saturation pressure (Pa)
R	Universal gas constant (J/kg-K)
Re	Reynolds number
<i>r</i> ₁ , <i>r</i> ₂	Radii of curvature (m)
r _i	Pore equivalent radius (m)
S	Arbitrary arc length (m)
$\langle S angle$	Average energy sink or source
Sc	Schmidt number
Т	Temperature (K)
$\langle T angle$	Porous medium average temperature (K)

\hat{T}	Dimensionless temperature
ΔT_{max}	Maximum temperature difference (K)
t	Time (s)
t _c	Critical time (s)
t_i	Time scale (s)
î	Dimensionless time
u	Velocity – x direction (m/s)
u_i	Velocity of ith species – radial r direction (m/s)
${U}_{\infty}$	Inlet air velocity (m/s)
V	Volume (m ³)
¥	Darcy's volumetric flow rate (m ³ /s)
\hat{V}	Dimensionless velocity
${ec V}_i$	Velocity vector of ith species (m/s)
W _i	Velocity of ith species – vertical z direction (m/s)

Greek Symbols

Buoyancy coefficient of temperature (1/K)	β
Buoyancy coefficient of concentration	β′
General transport coefficient	Γ
Thermogradient coefficient (1/°C)	δ
Luikov's phase change criterion	e
Volume fraction of the ith species	$\boldsymbol{\epsilon}_i$
Resistance to diffusion of a body	ζ
Normal directional vector	η
Bulk permeability of the ith species (m ²)	λ_i
Ideal minimum macro-pore size (m)	λ_{min}
Ideal maximum macro-pore size (m)	λ_{max}
Dynamic Viscosity (N-s/m ²)	μ
Dynamic Viscosity of ith species (N-s/m ²)	μ_i

Porous media topological function	ξ
Density (kg/m ³)	ρ
Spatial density (kg/m ³)	$\langle ho angle$
Volume averaged density of ith species (kg/m ³)	$\langle ho_i angle$
Surface tension (N/m)	$\sigma_{\beta\gamma}$
Dissipation function	Φ
General transport quantity	φ
Porosity	arphi
Liquid volume fraction	ψ
Capillary-diffusive parameter	Ω_eta

Subscripts

Solid phase	σ
Liquid phase	β
Liquid-gas interface	βγ
Gas phase	У
Main index	i
Secondary index	j
Time step index	k

Mathematical symbols

Partial derivative
Total derivative
Gradient/Divergence operator
Laplace operator
Summation

\int_{A}	Surface integral
\int_{V}	Volume integral
$\langle \rangle$	Phase average
$\langle \rangle^i$	Intrinsic phase average

1 Introduction

1.1 Problem Statement

Coffee is the world's most traded agricultural commodity. According to the ICO¹, it is produced in over 70 countries, employing approximately 25 million people. During the coffee year 2012-2013 the export was 113.157 million bags [1]. From this amount the exports of the species *Coffea Arabica* accounted for 72.69 %. Healthy coffee crops are usually observed in lands with a moderate temperature, good soil drainage, a soil pH of 4.0 to 7.0, and an annual rainfall that exceeds the 60 inches. The presence of these conditions makes tropical climate suitable for coffee production. Based on these environmental conditions, it is clear why the largest coffee producers are Brazil, Mexico and Colombia [2]. Most of the coffee growing countries have one major harvest per year. In the case of Puerto Rico, the coffee (*C. Arabica*) harvest season is between the month of August through January. Once picked, the coffee cherries must be processed for consumption. There are two common dehydration procedures: dry processing and wet processing. The dry method is used to obtain cherry coffee while the wet method is used to process parchment coffee [3].

Since our focus of interest is parchment coffee, fundamental knowledge of the wet processing concept is required. Processing is done immediately after the harvest. The coffee cherries are first sorted to determined if they meet the quality criteria. Then, the fruit surrounding the coffee seeds is removed. This process is often called "pulping" [5]. In spite of the fruit removal, a gluey mucilage layer will remain. To remove this coating of mucilage the bean is exposed to fermentation, since it will allow microbial decomposition of this layer [4]. The bean is then washed to remove any residual from the mucilage, or any debris. At the end of the cleaning process, the coffee bean has an average moisture content of 56%. To satisfy the corresponding regulatory agency (e.g. USDA) standards for coffee storage, the moisture content wet base (M.C. (w.b.)) of the bean must be in the range of 9 to 12 %. This level must be met to guarantee a high

¹ International Coffee Organization

quality coffee. The drying process is necessary to prevent deterioration due to bacteria and fungus growth on the grain. To prevent deformation of the bean due to shrinkage, it should not be dried below 9 % moisture [6]. Therefore, a proper dehydration process is required.

Small farmers dry coffee beans with direct solar energy, depending on climate conditions. However, this process is not adequate for large scale production due to quality and health concerns [7]. Thus, the usage of mechanical drying equipment is inevitable. The most common drying equipment used in Puerto Rico is the simple rotary-drum dryer. It consists of a perforated plenum chamber, one or several electric fans, and a combustion heater. During the traditional drying process, the hot air flows through the coffee mass, located inside of the chamber, removing water content from the beans and then the hot moist air exits the dryer. This process is continued until the hot air can no longer remove water from the coffee mass or the desired M.C. (w.b.) is met. To determine if the M.C. (w.b.) is in the range of 9%-12%, field tests are employed. The use of a rotary-drum dryer open system configuration entails high energy inefficiency. The use of a hot air recirculating controlled closed system (HARC²S) was proposed by Rodriguez et al.

1.2 Justification

Over the last few decades, the increase in the costs associated to fuel and electricity played a major role in the economic losses of the coffee industry. In Puerto Rico, the mean increasing rate of electricity from 1999 to 2012 was 8.44%. This situation represents an opportunity for the optimization of traditional drying equipment. The open rotary drum dryer used in Puerto Rico for the drying of parchment coffee is highly energy inefficient [8]. The employment of such inefficient equipment makes evident the lack of understanding of the mechanics behind the coffee dehydration process.

The dehydration process of a single coffee bean has been studied thoroughly [9, 30, 31]. For the drying process of different porous bodies, there are three usual stages observed. At the beginning of the process the body is saturated with water. Moisture migrates to the surface of the body driven by a significant concentration gradient. Once in contact with hot air, water is removed by evaporation. Since evaporation takes place only at the surfaces, the surface temperature decreases at a faster rate than the body temperature [10]. This phenomenon is often referred to as "evaporative cooling". Through the evolution of the evaporative cooling process, the evaporation rate decreases and the convective heat transfer increases until they reach equilibrium. When these phenomena, evaporative cooling and convective heat transfer, are at equilibrium, the removal of moisture is obtained at a constant temperature. The time lapse in which this intermediate stage takes place is determined by the convective heat transfer coefficient. In the last stage of this process, the moisture distribution inside the body becomes almost uniform. As a consequence, moisture migration becomes increasingly slower, while temperature increases asymptotically until equilibrium.

These characteristics have been observed and modeled for a single body. However, the actual drying process consists of a mass of many mutually interacting bodies. The latter stage observed for a single body just depends on temperature and concentration gradients between the porous solid and the hot air. It does not contemplate the effect of temperature and concentration gradients between one bean and another. One of the many disadvantages of the traditional open rotary-drum dryer is that temperature and moisture distribution of the coffee mass are not uniform [8]. At the latter stage, this implies an increase in the time required to reach equilibrium. Therefore, an analysis that includes the entire drying mass is required. With the information given by such model it will be possible to describe the conditions of the coffee mass through the entire process. This has the following advantages: (1) understanding the phenomenon a this level will help to optimize drying equipment and the parameters (airflow rate, temperature setting, etc.) of the process, (2) develop a prediction tool to help determine whether the desired M.C. (w.b.) has been reached. Therefore, the development of a constitutive model that describes the dynamics of parchment coffee during a typical dehydration cycle in an open system configuration and a HARC²S equipment is justified. The understanding of these dynamics will help to engineer highly energy-efficient coffee dehydrators.

1.3 Literature Review

The dehydration process was first analyzed as a heat and mass transfer problem in W.K. Lewis' work *The Rate of Drying of Solid Materials* [11]. He stated that this process consists on two principal stages: an initial stage in which the moisture migrates from the inside of the solid to the surface and a latter stage where the moisture is evaporated because of the heat received from an external source. This process was modeled as two independent phenomena. Hypothetically the early stage, often referred to as the funicular state, is driven particularly by a moisture concentration gradient. Once the distribution of moisture becomes uniform through the porous media, the drying process is dominated by convection and diffusion in the vapor phase. This latter stage is called by Haines [12] as the pendular state. Each state was analyzed by itself as an equally important contribution. Even though, the researchers rapidly move to give greater attention to the diffusion of liquid through the porous solid. An uneven approach like this is clearly shown in early works like those of Sherwood [13] and Newman [14]. Thus, their analysis was mainly based on Fick's laws of diffusion, stated as:

$$J = -D\frac{\partial C}{\partial x} \tag{1.1}$$

$$\frac{\partial C}{\partial t} = -D \frac{\partial^2 C}{\partial x^2} \tag{1.2}$$

As seen in the equations above, the diffusion is analyzed as an independent phenomenon, ignoring the codependency between diffusion and convection. The drying projections done with this assumptions represented good approximations for those scenarios in which the moisture content was relatively high. For those cases the variability due to temperature gradient were insignificant in comparison to the concentration gradient, which results in an almost constant drying rate. Gillilan & Sherwood [15] used the diffusion equation (Fick's second law of diffusion) to estimate the length of the "constant" rate of drying period. This length is limited by the critical free moisture content (X_c), which represented the minimum moisture required to

maintain a continuous film of water in the surface of the porous solid. Once the film is unattained, the effects of the convective interaction between the flow and the solid becomes unneglectable. At this point, the wetted surface area starts decreasing and the modeling of the dehydration process as a solely diffusion problem becomes totally inaccurate.



Figure 1.3.1: Batch Drying Rate Curve Under Constant Drying Conditions (from Mujumdar [16])

An improvement to the engineering analysis was obtained with the inclusion of the perspective of soil scientists and chemists. This resulted in new models that included the contribution of capillary forces in the moisture migration process. The work of Comings & Sherwood [17] sets an example of the influence of capillarity in the movement of moisture in porous media. As advanced as it was; the general knowledge of the dehydration processes was

limited by their analysis of heat and mass transfer as mutually exclusive phenomena. The concept of dealing with these two as a conjugated problem was first introduced by P.S.H. Henry [18]. He described the pores as a "continuous network of spaces included in the solid; containing the medium (e.g. air) through which the diffusion takes place". His conclusion was that; if vapor is absorbed by the solid when heat is added, then the vapor species will be set free by the solid when that heat is removed. Thus, diffusion is driven by simultaneously operating gradients of concentration and temperature. The former was a revolutionary addition to the contemporary thought of a non-interacting heat and mass transfer. Some refinements to this integrated heat and mass transfer model were done in the following decades. Philip and DeVries [19] related the diffusion mass flux to the volumetric moisture content gradient, the temperature gradient and the buoyancy forces contribution. Up to this moment, the contribution of each phenomenon was analyzed solely and then the individual effects were combined. This practice ignored the effects of a simultaneous exchange of heat and mass. With the physical knowledge of his predecessors; Luikov [20] established a coupled system of PDE for heat and mass transfer in porous bodies. Using Darcy's law he expressed conservation of mass and energy for a mixture of dry air and water vapor. This law, which is represented in the following constitutive equation, relates the volumetric flow through a porous medium with the viscosity of the fluid and the pressure drop. The permeability of the medium (K) establishes a relation between the fluid migration and the ability of a porous material to allow this fluid to pass through it.

$$\forall = \frac{-KA}{\mu} \frac{P_b - P_a}{L} \tag{1.3}$$

The equation above is manipulated an presented by Luikov & Mikhailov [21] in terms of the mass flow rate (*J*) and the dry-basis moisture content of the solid (ψ). This migration related to the pressure gradient is named "molar transfer" in Luikov's work.

$$J = \frac{\Psi}{\Psi + 1} \frac{K\rho}{\mu} \nabla P \tag{1.4}$$

While this "molar transfer" describes the mass diffusion through the pores, a general equation that applies at every point of the control volume had to be developed. The result was a system of non-linear equations, due to the integration of capillary forces, gradients and variable thermophysical properties as mutually inclusive driving forces of the drying process. Therefore, the transfer coefficients are represented as functions of either temperature or moisture content and the mass flux will depend on its gradients.

$$\boldsymbol{J} = \rho_0 \boldsymbol{a}_m (\nabla \boldsymbol{\psi} + \boldsymbol{\delta} \nabla T) \tag{1.5}$$

In the equation above, the diffusive mass flux is expressed as a combination of both phenomena using the density of the dry solid (ρ_0), the thermogradient coefficient (δ) and the moisture diffusivity (a_m). By substituting this expression into the differential energy and mass conservation equations it is possible to derive a system of equations that describes the simultaneous heat and mass transfer during the drying process of a porous body. This substitution is best known as *Luikov's System of Equations for Heat and Mass Transfer in Capillary-Porous Bodies*. If the effects of the gravitational force are neglected, it can be written as follows:

$$\rho_0 c \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + r \epsilon \rho_0 \frac{\partial \psi}{\partial t}$$
(1.6)

$$\frac{\partial \Psi}{\partial t} = \nabla \cdot (a_m \nabla \Psi) + \nabla \cdot (a_m \delta \nabla T)$$
(1.7)

where T is the temperature, ψ the moisture potential and c is the reduced specific heat. The reduced specific heat is given by:

$$c = c_0 + \sum_{i=1}^{3} c_i \psi_i$$
(1.8)

In this equation, c_i and ψ_i represent the specific heat and the mass content for phase *i*. In his work, Luikov uses the subscript *i*=0 referring to the solid body, *i*=1 for the vapor phase (including some inert gases) and *i*=2 for the liquid phase. Using these subscripts we could express the moisture content in the following form:

$$\psi = \frac{\sum_{i=1}^{2} m_i}{m_0} \tag{1.9}$$

To solve this complex system of equations, Luikov and Mikhailov [21] used the Laplace transform technique and assumed constant transfer coefficients. With their approach they obtained analytical solutions for the simple cases of a rod, a cylinder and a sphere. A different approach to this problem is presented by Whitaker [22], who proposed the usage of a volume averaged form of the transport equations. Although Whitaker and Luikov differed in their approaches their formulations are in agreement and most of the modern simplified models are based on these formulations. The governing equations presented in their work are similar; with the exception of the solid phase where Whitaker assumed the phase to be a dry solid, therefore ignoring the "bound moisture". This concept refers to a very thin layer of water that remains bounded to a solid surface due to the strong electrical polarity of water molecules. His approach consist of an application of the momentum principle and the thermal energy equation to describe the physical phenomena at every point in the control volume. Hence, an average between the governing equations of each separate phase is required. This method is helpful for an analytical study of a specific drying process without recurring into complex computational processes. With Withaker's approach starts an inclination to simplify the analysis within those coupled heat and mass transfer models.

The complexity of analyzing a non-isothermal process, such as the dehydration of a porous solid, impulsed the introduction of certain approximations in the usage of the basic conservation equations. An approximation commonly used to simplify the mass and momentum balances is attributed to Boussinesq [23]. This approximation is based on assuming that the density

differences are neglectable, and must be considered only in the calculation of buoyancy effects. For this reason, in the Boussinesq model, density is treated as a constant value in all the equations, except for the buoyancy term in the momentum equation. The buoyancy term is expressed in terms of the variable density ρ , which is a function of temperature, and the constant density ρ_0 . Boussinesq's approximation is written as follows:

$$\rho = \rho_0 (1 - \beta \Delta T) \tag{1.10}$$

$$\rho = \rho_0 (1 - \beta' \Delta C) \tag{1.11}$$

In the equations presented above, the complexity of using a variable density is reduced by introducing the buoyancy coefficient of temperature (β) and the buoyancy coefficient of concentration (β '). This simplification was implemented to analyze non-isothermal flows in the work of Rodi [24] and Shatzmann & Policastro [25]. The former work consists of a mathematical development of this approximation and a validation of non-Boussinesq and Boussinesq approximated models by comparison to experimental data from jet flow measurements. In the last years this approximation, like most of the approximations related to heat and mass transfer phenomena, had been reevaluated and compared with variable density models, as in the work of Geun & Kim [26], concluding that this approximation is acceptable for systems with symmetric density distributions. Even though, we must recall the importance of buoyancy and capillary forces in the concerning problem.

Merging all the concepts mentioned herein, several models had been developed concentrating efforts into the numerical solution of this conjugated problem. A one-dimensional model for simultaneous heat and moisture transfer was presented by Kallel [10]. In his work, which is mainly based on Withaker's theory of drying, he expressed the transfer coefficients as function of the moisture content. For this purpose, he stated that the vapor mass content was neglectable in comparison to the liquid mass content, thus it could be assumed that the moisture content was fundamentally equal to the liquid content. His approach was to independently calculate the mass transfer due to capillary forces and the mass transfer caused by the diffusion fluxes and then add

their contributions. The liquid mass flux due to capillarity was determined using Darcy's law in the following manner:

$$J_{c-l} = -\rho_l \frac{K_l}{\mu_l} \frac{\partial P_c}{\partial \eta}$$
(1.12)

$$\frac{K_l}{\mu_l} \frac{\partial P_c}{\partial \eta} = \frac{K_l}{\mu_l} \left(\frac{\partial P_c}{\partial \psi} \frac{\partial \psi}{\partial \eta} + \frac{\partial P_c}{\partial T} \frac{\partial T}{\partial \eta} \right) = D'_{ml} \frac{\partial \psi}{\partial \eta} + D'_{Tl} \frac{\partial T}{\partial \eta}$$
(1.13)

$$J_{c-l} = -\rho_o \left(D'_{ml} \frac{\partial \psi}{\partial \eta} + D'_{Tl} \frac{\partial T}{\partial \eta} \right)$$
(1.14)

In these expressions the flux is determined based on the respective capillarity isothermal mass transfer coefficient (D'_{ml}) and non-isothermal mass transfer coefficient (D'_{Tl}) . The density of the liquid and the density of the air are represented as ρ_1 and ρ_0 respectively. Similarly, the mass transfer caused by diffusion was determined applying a modified version of Fick's law. This modification consists of correcting the diffusion flux to account for the resistance to diffusion (ζ) inside the porous body, which is stated as dependent of the moisture content.

$$J_{d-w} = -\zeta D_j \frac{\partial C_j}{\partial \eta}$$
(1.15)

$$J_{d-w} = -\rho_o \left(D''_{ml} \frac{\partial \psi}{\partial \eta} + D''_{Tl} \frac{\partial T}{\partial \eta} \right)$$
(1.16)

Combining the mass transfer caused by each phenomenon it is possible to express the total flux as function of both moisture content and temperature. Substituting the following equation into our constitutive equations makes possible to express the dehydration process as a conjugated problem.

$$J_{w} = -\rho_{o} \left(D_{ml} \frac{\partial \Psi}{\partial \eta} + D_{Tl} \frac{\partial T}{\partial \eta} \right)$$
(1.17)

This equation is another form of the diffusive mass flux equation for the liquid phase Eq (1.5). Using the same approach its possible to establish the diffusive mass flux equation for the vapor phase. To numerically solve the obtained equations, Kallel discretized the equations explicitly using the finite difference method and expressed the boundary conditions in a steady state form. The difference from his results and measured values was relatively small for the cooling-down or evaporative cooling period (phase 1), which is the first stage in a dehydration process. For the constant temperature period (phase 2), he had some significant differences which could be attributed to the usage of a constant convection coefficient.

Using a similar approach, Murugesan & et al. [27] develop a two-dimensional model to describe the process of brick drying. The governing equations were expressed using the same method as Kallel; defining the mass flux in terms of moisture content and temperature by the usage of transfer coefficients. As usual, these coefficients were determined from correlations obtained using boundary layer equations. To solve the coupled equations numerically, Murugesan used finite element spatial discretization applying Galerkin's weighted residual method. Again, steady flow was assumed and pressure terms in the x and y momentum equations were neglected due to the complexity of the problem. An extensive analysis of the heat and mass transfer interactions was possible in this work by means of monitoring changes in Nusselt and Sherwood number through the geometry of the solid. The results were congruent with those from Kallel, making evident the existence of the three phases of the dehydration process. Even though, its necessary to point out that the attributes of these phases will vary from one material to another.

Another two dimensional model for conjugate heat and mass transfer in porous body is presented by Amanifard & Haghi [28]. They linked several of the concepts mentioned before such as Boussinesq approximated model and the usage of a total mass flux based on transfer coefficients to deal with the inhomogeneity of the phenomena. Using Boussinesq's approximation they coupled the different transfers into the momentum equation of the flow field.

$$\frac{Du}{Dt} = -\frac{1}{\rho} \frac{\partial P}{\partial x} + v \nabla^2 u \tag{1.18}$$

$$\frac{Dv}{Dt} = g \beta (T - T_{\infty}) + g \beta' (C - C_{\infty}) - \frac{1}{\rho} \frac{\partial P}{\partial y} + \frac{\mu}{\rho} \nabla^2 v$$
(1.19)

To consider coupled heat and mass transfer in the governing equations of the porous solid, they used the isothermal and non-isothermal mass transfer coefficients for the moisture content. Thus, for incompressible flow and constant thermophysical properties, conservation of energy and mass are expressed in terms of these transfer coefficients as follows.

$$c\frac{\partial T}{\partial t} = \left(\frac{k}{\rho_o} + h_{fg} D_{tv}\right) \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right) + h_{fg} D_{mv} \left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2}\right)$$
(1.20)

$$c = c_o + m_l c_l + m_v c_v \tag{1.21}$$

$$\frac{\partial \psi}{\partial t} = (D_{tl} + D_{tv}) \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right) + (D_{ml} + D_{mv}) \left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2}\right)$$
(1.22)

Some three-dimensional models had been developed recently with the general purpose of visualizing certain patterns on the drying process in porous media, specifically to characterize the saturation profile and identify the different stages in the drying curves. Le Bray and Prat [29] pore network simulation modeled the solid as a simple cube lattice with randomly located voids of various sizes; the sizes were given using an uniform distribution with an average width of 0.4 mm. In their work, they considered the capillarity effects, the phase change at the liquid-gas interface and diffusion in the gaseous phase. To calculate the mass transfer at the surface of the solid, a local constant mass transfer coefficient was used. The drying curves obtained were in qualitative agreement with experimental results, but they clearly stated that the results were preliminary and that, due to the complexity and time demand, the heat and mass transfer transport equations were solved as a non-conjugated problem.

Most of the works mentioned herein do not agree in their approaches but almost all of them emphasize in the importance of the transfer coefficients to couple heat and mass transfer as an integrated problem. Here is where the physical model relies in the data available from past experiments. Thus, to accurately model this phenomena we must refer to the experimental work done using the specific porous material to be studied. Then, it is our concern to review the research work done on the drying process of wet parchment C. arabica. In the work of Pérez-Alegría [30], the behavior of physical and thermal properties was estimated as a function of moisture content. Geometrical parameters of the parchment coffee bean, such as length, width, and thickness were measured. The specific heat was calculated using the method of mixtures; which assumes ideal experiment conditions; all the heat lost by the coffee bean is received by the surrounding fluid and the calorimeter. To calculate the bulk thermal conductivity, the line heat source method was applied obtaining a linear relation between conductivity and moisture content. The values of specific heat obtained were greater than the data available for similar beans, while the thermal conductivity was smaller. This implies that the drying processes.

Another important parameter to consider is the diffusion coefficient. This coefficient will vary depending on whether the selected location is within the lattice or at the grain boundary. The usual procedure is to take an average between both coefficients. This average is called the effective diffusivity coefficient *D*. According to Corrêa [31] the influence of temperature in this coefficient could be represented as an Arrhenius relation.

$$D = D_0 \exp\left(\frac{-E_a}{RT_a}\right) \tag{1.23}$$

In the equation above D_0 is the pre-exponential factor, E_a is the activation energy, R is the universal gas constant and T_a is the temperature of the air. Using experimental measurements of moisture content they were able to determine an experimental effective diffusivity coefficient. This was possible by evaluating an analytical solution of Fick's second law for the coffee fruit

drying process. In our case *C* represents the concentration of water or moisture content inside the coffee cherry.

$$\frac{\partial C}{\partial t} = D \nabla^2 C \tag{1.24}$$

For a single grain; assuming azimuthal and zenithal symmetry, and neglecting the shrinkage effects of dehydration the solution of the former equation yields to:

$$MR = \frac{6}{\pi^2} \sum_{1}^{\infty} \frac{1}{n^2} \exp\left(\frac{-n^2 \pi^2 Dt}{r^2}\right)$$
(1.25)

Where the moisture rate (*MR*) is defined in terms of the initial moisture content (C_i), the equilibrium moisture content (C_e) and the actual moisture content (C).

$$MR = \frac{C - C_e}{C_i - C_e} \tag{1.26}$$

A proper relation was determined by comparing the experimental coefficients obtained through this method with the Arrhenius equation. For the parchment *C. arabica*, Corrêa reports a pre-exponential factor of $2.041 \cdot 10^{-6}$ m²s⁻¹ and a water activation energy of 22.619 kJ/mol. With the former knowledge and applying principles of energy and mass conservation, some engineering models had been developed as prediction tools for coffee processors. Perez-Alegria [7] adapted Bakker-Arkema model for grain drying in deep beds to describe the airflow reversal drying process of parchment coffee. The Bakker-Arkema model describes simultaneous heat and mass transfer by applying the concepts of sensible and latent energy. The former was modified by including a thin-layer relationship. Rodriguez-Robles [51] presented a parametric thermodynamic model to predict the behavior of both temperature and moisture content through the dehydration process of parchment coffee beans. This model consists of a formulation of the first law of

thermodynamics; accounting for sensible and latent energy. Including the latent energy, both energy and mass equations were coupled. This work shows the advantage of using a coupled system of equations to describe this phenomenon by obtaining less than 2% of error between the thermodynamic model and the experimentally collected data.

As stated through this review, the modeling of a dehydration process is not trivial. It requires an understanding of the driving forces, the conditions of the specific process and the governing principles. In our case, the drying of wet parchment *C. arabica* has been modeled for multidimensional simplified cases or parametrically. Even when parametric models, which analyze the input and the output independently of the system, give useful results there is still a gap in the understanding of this process. If we add to our problem the consideration of micromacro pore interactions, irreversibility of the process and try to develop a transient 3-D model, we will see that there is still room for improvement in our actual models.

1.4 Objectives

In order to reduce the energy inefficiencies associated with the dehydration process of wet parchment coffee (*C. arabica*) in the traditional rotary drum dryers, this drying process must be described both physically and mathematically. Formulating a mathematical model will improve our understanding of the thermodynamic characteristics of this process. It will allow us to predict the temperature and M.C. (w.b.) distributions throughout the coffee mass during the dehydration process. Furthermore, the development of accurate heat and mass transfer mathematical models will allow for parametric optimization of the drying equipment. The proposed research effort seeks to enhance the understanding of the dehydration process of wet parchment coffee (*C. arabica*). Specific objectives are to:

 Develop a mathematical constitutive model that will predict the temperature and M.C. (w.b.) for the dynamics of parchment coffee mass during the dehydration cycle using rotary drum technology. 2. Calibrate the mathematical constitutive model with published and/or measured experimental data.

The expected outcomes for the proposed research effort are as follows:

- **1.** Obtain a precise understanding of the thermodynamics surrounding the dehydration process of the parchment coffee mass.
- 2. Predict the dynamics of dehydration via the use of the developed mathematical model.

1.5 Materials and Methods

The methodology to be used will be divided into four general steps: (1) formulation, (2) modeling, (3) data collection and (4) calibration. The formulation of the drying phenomena within the coffee mass will be done using the equations of energy and mass transport. The drying process will be analyzed at two different scales: macro-pore level and micro-pore level. The macro level considers the motion of moist air through the coffee mass. At this level its possible to describe the moisture removal by generalizing the coffee mass as a single porous body. The micro level considers the migration of water and vapor through a single coffee bean. With the combination of these formulations we can describe the entire moisture transport phenomenon.

Once the problem is well posed, the solution will be determined for different cases. It will be done starting from the simplest case of one-dimensional steady state conditions, moving towards the complete multi-dimensional case. Due to the complexity of the problem, most of these solutions will be numerically obtained. This progressive approach will be essential to determine the dependencies of the phenomenon. An appropriate parametric model will be proposed based on this information. The following step will be to calibrate the obtained model using experimental data. Experimentation will be done using a hot air recirculation controlled-closed system (HARC²S). This system was designed and constructed by Dr. Francisco Rodríguez Robles and Dr. Francisco Monroig Saltar from the University of Puerto Rico at Mayagüez. The HARC²S (*Figure 1.2*) is an alternate dryer designed to decrease the energy consumption during the drying process by recirculating and reconditioning the dehumidifying hot air. "The hot and humid air passing through the parchment coffee material is directed to a HX device where a portion of the moist air water content will be condensed and collected outside the dehydration cycle with minimum recirculating hot air temperature drop. The dehumidified air will recirculate back into the heating source where it will be heated back to the dehydration temperature setting of the equipment [2]."

This system will be instrumented with HOBO Pro V2 temperature and relative humidity sensors (*Figure 1.3*) to monitor moist air dry bulb temperature, relative humidity and coffee mass temperature. These sensors will be set to take measurements at a sample rate of once per minute. The saturated coffee mass will be exposed to a complete drying cycle. Every 30 minutes a sample will be taken out of the drying chamber. Then, the M.C. (w.b.) of the sample will be determined by loss of weight on heating, which is the accepted standard method [6]. For this purpose we will use a calibrated Denver Instrument IR-35 Moisture Analyzer (*Figure 1.4*). Once the moisture level of the sample reaches 12 % the drying process will be finished. The collected data will be evaluated and compared with the predictions done with the proposed model. Using these measured experimental results will serve to calibrate the mathematical constitutive model.





Figure 1.5.1: HARC²S Device



Figure 1.5.2: HOBO Pro V2 Sensor



Figure 1.5.3: IR-35 Moisture Analyzer

1.6 Thesis Structure

This study presents the development of a mathematical model for the dehydration process of parchment coffee (*C.Arabica*). In Chapter 2 an overview of the mathematical method, its assumptions, constraints and physical significance is presented. At the end of this chapter, a summary of the model is presented and once again the non-linearity of the equations used is highlighted. This system of equations requires a numerical method, a proper selection of boundary conditions and a solution strategy based on the phenomenology behind this model. Chapter 3 is devoted to the discussion of this method. It includes a brief introduction to the finite volume method, an explanation of the discretization schemes used, a dimensionless study of the system of equations and the development of a convergence strategy based on this dimensionless study. In Chapter 4 the results obtained with this model are presented and compared with measured experimental data. The error of the model is characterized and described by simple statistics. In Chapter 5 the conclusions and proposed future work to improve the model are presented. There, the probable sources of error are discussed as well as the strengths of the model.

2 Mathematical Modeling

This study considers the motion of liquid water, water vapor and dry air through a rigid porous body (parchment coffee *C.Arabica*). Water and its vapor migrate through single coffee bean pores (micropore level) due to the gradient of transport quantities (temperature and mass). In the void space created between beans (macro-pore level) the water is removed by the combination of vaporization and convection. Although the concept of funicular and pendular states was introduced earlier (section 1.3), it is necessary to explain their physical significance since these will be often mentioned in this study. In the earlier stage (funicular) of the dehydration process the porous media is saturated and the phase change (vaporization) will have a stronger effect on transport quantities than other transport mechanisms. The pore channels are filled with water at this stage, hence the liquid water will travel to the surface of the coffee beans by capillary action. Once the saturation level decreases substantially, the vaporization rate will also decrease. This event announces the transition into the secondary stage of the process, in which the migration of liquid occurs due to mass diffusion (concentration gradients) and convection-diffusion is the principal source of transport. Both stages are illustrated in *Figure 2.1*.



Figure 2.1: Dehydration Process Characteristics
To characterize this dehydration process we desire to determine the moisture content and temperature as a function of time and space. As illustrated above, to do this we must study the transport of energy and mass taking place between the different phases included in our studied volume. This analysis must consider both the microscopic and macroscopic scale. In the selected nomenclature the σ phase represents the solid porous matrix, β phase consists of liquid water (no bubbles) and γ is our gas phase, which consists of moist air (dry air and water vapor). The governing equations of these transport phenomena will describe the physical processes at a certain point within one of the zones or phases. For that reason it will be referred to this system of equations as zonal governing equations.

2.1 Zonal Governing Equations

2.1.1 Solid Phase (σ)

The solid phase consists of a rigid solid matrix of parchment coffee beans of the species *C.Arabica*. This solid matrix is assumed to be homogeneous, but anisotropic (spatial variation of thermo-physical properties). It is considered to be fixed to the coordinate system, which implies that the velocity of the σ phase is zero. Applying the law of conservation of energy, it yields the following energy equation in which the change in energy is purely attributed to the mechanism of diffusion (conduction).

$$\rho_{\sigma}C_{p-\sigma}\frac{\partial T_{\sigma}}{\partial t} = K_{\sigma}\nabla^{2}T_{\sigma}$$
(2.1)

In the equation above the thermal conductivity and specific heat of the σ phase are consider to be constant. Still, in the solution of these equations these properties could be evaluated as spatial averaged values to improve the accuracy of results. If we apply the law of conservation of mass to the solid phase the yielding result is redundant, since the solid mass remains constant and bounded moisture is neglected.

2.1.2 Liquid Phase (β)

The β phase consists of liquid water and it is the phase that changes most throughout the dehydration process. At the beginning of the process this phase is partially continuous (continuous inside the pore volume). As the coffee mass moisture content decreases this phase becomes discontinuous until the number of discontinuities becomes very large; it is to say that the discontinuities of β phase becomes infinite as the porous media becomes completely dry. Applying the law of conservation of energy it is determine that the local increase of energy (zonal rate of change) at this phase must be equal to the the difference between the incoming diffusion energy (via conduction) and the dissipation of energy due to advection.

$$\rho_{\beta}C_{p-\beta}\left(\frac{\partial T}{\partial t} + \vec{V}_{\beta} \cdot \nabla T_{\beta}\right) = K_{\beta} \nabla^2 T_{\beta}$$
(2.2)

If we also evaluate the conservation of mass (continuity) in the liquid phase, recalling that liquids such as water are assumed incompressible fluids, we can say that the local increment in mass must be equal to the mass flux incoming to the system. This is not true at the liquid-gas interfaces (β - γ discontinuities), where we must also include the mass flux due to phase change (vaporization or condensation). Since this is a zonal equation, any phase change is not taken into account. As will be seen later, the vaporization-condensation fluxes will be considered as discontinuous phenomena. Thus we can write our zonal β phase continuity equation as,

$$\frac{\partial \rho_{\beta}}{\partial t} + \nabla \cdot \left(\rho_{\beta} \vec{V}_{\beta} \right) = 0$$
(2.3)

2.1.3 Gas Phase (γ)

The gas phase consists of the water vapor and dry air. It is important to point out that no chemical reaction occurs in the gas phase, since the dry air is inert. Also, the dry air does not interfere in the phase change, since it is insoluble in water (β phase). Something that must be understood before formulating the energy equation for this phase is that the total energy equals the sum of the energy of

the individual species, but the total energy flux is not equal to the sum of the fluxes of the individual species. This can be illustrated with the following expressions.

$$\rho_{\gamma} h_{\gamma} = \sum_{i=1}^{i=N} \rho_i \bar{h}_i$$
(2.4)

$$\rho_{\gamma}\vec{V}_{\gamma}h_{\gamma} \neq \sum_{i=1}^{i=N} \rho_{i}v_{i}\overline{h}_{i}$$
(2.5)

The reason for this inequality is that the total velocity of the phase depends not only on the species velocity v_{i} , but also depends on the diffusion velocity of the species u_i (Eq. 2.6). This diffusion velocity can be easily related to the gradient of the concentration of the *i* species using Fick's law (Eq 2.7).

$$v_{\gamma} = v_i - u_i \tag{2.6}$$

$$\rho_i u_i = -\rho_{\gamma} D_i \nabla \left[\frac{\rho_i}{\rho_{\gamma}} \right]$$
(2.7)

Using the law of conservation of energy, the resultant zonal energy equation is

$$\rho_{\mathbf{y}} (C_p)_{\mathbf{y}} \left(\frac{\partial T_{\mathbf{y}}}{\partial t} + \vec{V}_{\mathbf{y}} \cdot \nabla T_{\mathbf{y}} \right) = K_{\mathbf{y}} \nabla^2 T - \nabla \left(\sum_{i=1}^N \rho_i \bar{u}_i \bar{h}_i \right)$$
(2.8)

Similar to the zonal energy equation of liquid phase, the local change of energy of the γ phase is equal to the energy gain via conduction minus the energy removed due to convective transport. The difference here, as we can see from the right side of Eq. (2.8), is that some energy is removed (or acquired) due to concentration gradients. Again, the thermophysical properties are assumed to be constant in the selected differential volume. When applying the conservation of mass principle, we will find that the local change of mass must be equal to the net mass flux entering our control volume (Eq. 2.9). To be consistent with liquid phase zonal transport equations, any phase change will be assumed to take place at the liquid-gas interfaces (β - γ discontinuities).

$$\frac{\partial \rho_{\gamma}}{\partial t} + \nabla \cdot \left(\rho_{\gamma} \vec{V}_{\gamma} \right) = 0$$
(2.9)

This set of equations describe the phenomena in terms of the individual phases, but it makes impossible to find a solution; since this will be highly influenced by the discontinuity terms at the interfaces σ - β , β - γ and σ - γ . To formulate a system of equations valid at any point in space, a volume averaged form of these equations, derived by Whitaker [22], will be used.

2.2 Volume Average Method

To illustrate the volume average technique lets consider the porous media presented in Figure 2.2.1.



Figure 2.2.1: Porous Media (with Discontinuous Liquid Phase)

To introduce this method first it is necessary to understand the difference between spatial, phase and intrinsic phase averages. The first one (Eq. 2.10) refers to the average of a quantity defined everywhere in our control volume of volume V. The phase average (Eq. 2.11) is the average of a transport quantity defined only in one phase with respect to the total volume V. An intrinsic phase average (Eq. 2.12) is the average of a quantity defined only in one phase with respect to the total volume V. An intrinsic phase average (Eq. 2.12) is the average of a quantity defined only in one phase with respect to the volume occupied by that same phase. The understanding of these differences is vital in the formulation of the volume averaged transport equations for our dehydration process.

$$\langle \psi \rangle = \frac{1}{V} \int_{V} \psi \, dV \tag{2.10}$$

$$\langle \Psi_i \rangle = \frac{1}{V} \int_V \Psi_i dV \tag{2.11}$$

$$\langle \psi_i \rangle^i = \frac{1}{V_i} \int_{V_i} \psi \, dV \tag{2.12}$$

In spite of the fact that it is not the scope of this study to derive the volume averaged theorem or the averaged transport equations, we may discuss some details about this method for its physical implications. For a detailed derivation of the averaging theorem, see the work of Slattery [32]. One of the challenges of formulating a system of volume averaged transport equations is relating the average gradient of a transport quantity to the average of the quantity itself. A useful expression is developed using the so-called averaging theorem . This theorem states that the average of a quantity's gradient is equal to the gradient of the quantity's average plus the average of the quantity jumps (discontinuities) at interfacial areas between different phases. In terms of the problem presented herein, we can say that the volume average of any transport quantity's derivative could be represented as the derivative of that quantity's average plus the average jump of the quantity at the interfaces σ - β (solid-liquid), β - γ (liquid-gas) and σ - γ (solid-gas). This can be mathematically expressed for a transport property at phase *i* as

$$\langle \nabla \psi_i \rangle = \nabla \langle \psi_i \rangle + \frac{1}{V} \sum_{j=1}^N \left(\int_{A_{i-j}} (\psi_i - \psi_j) \cdot \eta_{i-j} dA \right)$$
(2.13)

The first term at the right side of Eq. (2.13) represents the gradient of the average of the transport quantity ψ_i and the second term represents the jump of this quantity at the interface *i-j*. To deal with these discontinuity terms we'll need to either employ a constitutive equation or use some physical deduction to understand the significance of the term. This terms represents one of the biggest complexities in the modeling of transport phenomena in porous media and also a common source of error. Utilizing the averaging theorem and some constitutive equations, the average form of the transport equations is formulated. In the following section, a descriptive flowchart of the formulation

process is presented.

2.3 Methodology – Flowchart

In the diagram depicted in Figure 2.3.1 the process of formulating the volume averaged transport equations for a porous media is illustrated.



Figure 2.3.1: Formulation of Volume Averaged Equations

The first step is to add the zonal equations presented in section 2.1 and simplify the resulting expressions using the averaging theorem. This would lead to an early form of the volume averaged

equations. Contained in this expressions we will find average terms (which are usually the desired averaged transport quantities), jump discontinuity terms and dispersion terms which are usually the nonlinear terms resulting from averaging convective (non-linear) terms in the transport equations. Jump discontinuity terms are usually eliminated by using some constitutive equation and terms containing the dispersion vector are either related to the tortuosity vector (if known), determined experimentally or combined into effective parameters (e.g. effective diffusion coefficient). In the expressions presented by Whitaker [22] the dispersion vectors are combined into effective transport coefficients. A detailed analysis of the dispersion vector and its relation to the tortuosity vector is presented by Whitaker [33].

2.4 Assumptions and Limitations of Methodology

Before presenting the averaged continuum equations, the assumptions and restrictions of our model must be clear. Some assumptions have been already introduced but all are summarize here to keep a coherent structure in our discussion.

Assumption 1: The solid matrix is fixed to our coordinate system

$$\vec{V}_{\sigma} = 0 \tag{2.14}$$

This represents a limitation in terms of the physical understanding of our dehydration process, since in the actual conditions of the dehydration process of parchment coffee the coffee is being stirred by a lever arm.

Assumption 2: The thermal conductivities of σ , β and γ phases are constant in the differential volume. **Assumption 3:** The enthalpies of σ , β and γ phases are independent of pressure and the specific heats are all constants inside the differential volume.

$$h = h(T) = C_p + const \tag{2.15}$$

To specify that the enthalpy is independent of pressure, not only implies that it is a unique function of internal energy but also that the compressional work is negligible.

Assumption 4: β (liquid) phase is pure.

Assumption 5: Viscous dissipation is negligible

$$\Phi_{dissipation-\beta} = \Phi_{dissipation-\gamma} = 0 \tag{2.16}$$

Assumption 6: The change in kinetic and potential energy of β and γ phases is zero.

Assumption 7: There is no chemical reaction in the γ phase.

As stated before, the dry air is inert and insoluble in σ and β phases.

Assumption 8: The γ (gas) phase is ideal.

This assumption will be substantial, specially at the formulations of vapor pressure and intrinsic phase density.

Assumption 9: The flow is quasi-steady.

$$\frac{\partial \vec{V}_{\beta}}{\partial t} = \frac{\partial \vec{V}_{\gamma}}{\partial t} \approx 0 \tag{2.17}$$

The characteristic time of most dehydration processes is big enough to treat the flow as quasi-steady. While calculating the different time scales (Sections 3.2.4, 3.2.5) it will be shown that this is true for this specific process. Another calculation that will support this assumption is the estimate of Reynolds number. Due to the resistance that the parchment coffee bed (porous body bulk mass) represents, the flow is expected to be in Darcy regime (Re < 1). This will be discussed further in Section 3.2.3.

Assumption 10: The σ (solid), β (liquid) and γ (gas) phases are assumed to be in local thermal equilibrium. This will be explained with further detail in section 2.5.1.

Assumption 11: The β and γ phases are Newtonian fluids with constant viscosity. This assumption eliminates the possibility of studying the presence of certain oils in our porous media.

Assumption 12: The gas phase is continuous.

Assumption 13: The gas and liquid pressure distribution are hydrostatic.

Assumption 14: The capillary pressure is a unique function of phase average temperature and liquid phase volume fraction.

$$\langle P_c \rangle = f(\langle T \rangle, \epsilon_{\beta})$$
 (2.18)

$$\langle P_c \rangle = -\frac{1}{A_{\beta\gamma}} \int_{A_{\beta\gamma}} \sigma_{\beta\gamma} \left(\frac{1}{r_1} + \frac{1}{r_2} \right) dA$$
 (2.19)

It is known, from Young-Laplace equation (Eq. 2.19), that the capillary pressure is a function of the surface tensions and the radii of curvature. Therefore, this assumption implies that the surface tension and radii of curvature are also functions of temperature and liquid phase volume fraction.

2.5 Continuum Averaged Equations

The averaged equations presented here are derived with detail in Slattery [32], Gray [34] and Withaker [22].

2.5.1 Total Thermal Energy

The transport of heat and mass in porous media is usually characterized by having relatively low convective heat transfer rates [22, 35]. This could be physically deducted since porous media flows are generally in the Darcy regime and, in average, the volumetric resistance to heat transfer prevails over the surfaces resistance. Therefore, we can assume that the σ , β and γ phases are in local equilibrium and the intrinsic phase average temperatures are all the same temperature $\langle T \rangle$.

$$\langle \rho \rangle c_{p} \frac{\partial \langle T \rangle}{\partial t} + \left[\rho_{\beta}(c_{p})_{\beta} \vec{V}_{\beta} + \langle \rho_{\gamma} \rangle^{\gamma} \langle c_{p} \rangle^{\gamma} \langle \vec{V}_{\gamma} \rangle \right] \cdot \nabla \langle T \rangle =$$

$$\nabla \cdot \left[K_{eff} \nabla \langle T \rangle \right] - \langle \dot{m} \rangle \Delta h_{vap}$$

$$(2.20)$$

The equation above represents total thermal energy of our solid-liquid-gas system. It states that the

local change of energy must compensate for the incoming diffusive energy fluxes, the exiting convective energy fluxes and the energy spent in the vaporization of water.

2.5.2 γ-phase Continuity

The following equation represents the mass continuity of the gas phase. Physically, it means that the change in mass per unit volume of the gas phase is equal to the incoming water vapor (due to vaporization phenomenon) minus the flux of gas leaving the differential volume.

$$\frac{\partial \left(\epsilon_{\gamma} \langle \rho_{\gamma} \rangle^{\gamma}\right)}{\partial t} + \nabla \cdot \left(\langle \rho_{\gamma} \rangle^{\gamma} \langle \vec{V}_{\gamma} \rangle\right) = \langle \dot{m} \rangle$$
(2.21)

As we can see in the last equation, the average mass per unit volume of gas is written as the product of the gas phase volume fraction (ε_{γ}) and the intrinsic phase average density. It is essential to clarify that the intrinsic phase average density of the different species in the gas phase is different to the phase average.

$$\langle \rho_i \rangle^{\gamma} = \frac{1}{V_{\gamma}} \int_V \rho_i dV \neq \frac{1}{V} \int_V \rho_i dV$$
 (2.22)

$$\langle \rho_i \rangle^{\gamma} = f(\langle T \rangle, \epsilon_{\gamma})$$
 (2.23)

The intrinsic phase average is both a function of the phase average temperature and the space occupied by the gas phase (γ volume fraction). For this reason the density used in this equation cannot be evaluated from thermodynamic correlations based on phase average temperature. In the latter stage of the process, when the coffee mass is not saturated anymore, we can say that the gas occupies all the space between coffee grains and the intrinsic phase average will be function of temperature and bulk porosity.

2.5.3 β-phase Continuity

The volume averaged β -phase continuity equation is presented in Eq. (2.24). This expression states that the change (reduction) in the volume occupied by the liquid water (ϵ_{β}) must equal the water evaporating plus the water exiting the differential volume in liquid form.

$$\frac{\partial \epsilon_{\beta}}{\partial t} + \nabla \cdot \langle \vec{V}_{\beta} \rangle + \frac{\langle \dot{m} \rangle}{\rho_{\beta}} = 0$$
(2.24)

In the expression above we can see how the intrinsic phase average water density has been replaced by its phase average. The reason for this substitution is that liquid water is an incompressible fluid. Consequently, an increment in the water content will be instantaneously followed by an increment in the water volume fraction.

2.5.4 γ-phase Motion

As discussed in section 2.4, the porous media flow is characterized by very low speeds. For this reason we will treat the gas velocity as a quasi-steady quantity (local change in time is negligible).

$$\langle \vec{V}_{\gamma} \rangle = -\left(\frac{\lambda_{\gamma}}{\mu_{\gamma}}\right) \left[\vec{\nabla} \langle P_{\gamma} - P_{0} \rangle^{\gamma} - \rho_{\gamma} \vec{g} \right]$$
(2.25)

This vector equation is a form of Darcy's law; where λ_{γ} represents the permeability tensor and μ_{γ} is the dynamic viscosity tensor. For the solely development of this equation the flow was treated as incompressible although some variations in the density are expected. An assumption implemented here is that the gas phase is always continuous. This represents a limitation specially at the early stage of the dehydration process when we expect the gas phase to be discontinuous and its density will vary due to the presence of liquid water.

2.5.5 β-phase Motion

The approach Whitaker [22] proposed to model the motion of water in porous media is to assume that the liquid flow depends only on gravity and capillary forces. Gravity force is represented by the hydrostatic pressure and the capillary force is represented by the capillary pressure. The former is a function of the surface tension forces and the radii of curvature at the gas-liquid interfacial area (discontinuities). Based on this, the following expression for the motion of β phase is developed.

$$\langle \vec{V}_{\beta} \rangle = -\left(\frac{\xi \lambda_{\beta} \epsilon_{\beta}}{\mu_{\beta}}\right) \left[\nabla P_{c} + \left[\rho_{\beta} - \rho_{\gamma} \right] \vec{g} \right]$$
(2.26)

As we can see the equation above is a form of Darcy's law. In this expression we state that the flow of water is proportional to the pressure drop due to capillarity minus the gravitational potential of the liquid phase relative to the gas phase. This equation introduces the parameter ξ , which is a function of the topology of the liquid phase. When ξ equals 1, the equation above becomes Darcy's law. This represents the case where β phase is totally continuous and the only discontinuity is the boundary enclosing it. Similarly the magnitude of the liquid motion decreases to zero as ξ becomes 0. This represents the case where the number of discontinuities goes to infinity. Therefore, we can say that the topological parameter ξ is inversely proportional to the number of phase discontinuities *M*.

$$\xi \propto \frac{1}{M} \tag{2.27}$$

One of the problems of this methodology is determining this parameter, which could be extracted from the experimental deduction of the saturation curves. In our modeling, this parameter will be related to the volume fraction of liquid phase (Section 2.6.8). Now, we still have to model or determine the capillarity pressure in terms of our transport quantities. This will be done assuming that the pressure is a unique function of temperature and volume fraction. Thus, the capillary pressure gradient can be written as

$$\vec{\nabla} \langle P_c \rangle = -k_{\epsilon} \vec{\nabla} \epsilon_{\beta} - k_{\langle T \rangle} \vec{\nabla} \langle T \rangle$$
(2.28)

Introducing Eq. (2.28) into Eq. (2.26) we obtain:

$$\langle \vec{V}_{\beta} \rangle = -\left(\frac{\epsilon_{\beta} \xi \lambda_{\beta}}{\mu_{\beta}}\right) \left[k_{\epsilon} \vec{\nabla} \epsilon_{\beta} + k_{\langle T \rangle} \vec{\nabla} \langle T \rangle - \left[\rho_{\beta} - \rho_{\gamma}\right] \vec{g}\right]$$
(2.29)

where

$$k_{\epsilon} = -\frac{\partial \langle P_c \rangle}{\partial \epsilon_{\beta}}, \qquad k_{\langle T \rangle} = -\frac{\partial \langle P_c \rangle}{\partial \langle T \rangle}$$
(2.30)

The parameters presented in Eq. (2.30) can be determined from an experimental curve relating the capillary pressure to the liquid saturation level. However, in our study of the drying process of parchment coffee, we will represent this parameters with the following expressions.

$$k_{\langle T \rangle} = -\frac{\partial \langle P_c \rangle}{\partial \langle T \rangle} = -\frac{\partial \langle P_c \rangle}{\partial \sigma_{\beta \gamma}} \frac{\partial \langle \sigma_{\beta \gamma} \rangle}{\partial \langle T \rangle}$$
(2.31)

$$k_{\epsilon} = -\frac{\partial \langle P_{c} \rangle}{\partial \epsilon_{\beta}} = -\frac{\partial \langle P_{c} \rangle}{\partial \sigma_{\beta\gamma}} \frac{\partial \langle \sigma_{\beta\gamma} \rangle}{\partial \langle T \rangle} \frac{\partial \langle T \rangle}{\partial \epsilon_{\beta}}$$
(2.32)

The expressions above assume again that the surface tension is a unique function of temperature and that the radii of curvature is constant. Therefore, Young-Laplace equation reduces to

$$\langle P_c \rangle = -\frac{2}{A_{\beta\gamma}r} \int_{A_{\beta\gamma}} \sigma_{\beta\gamma} dA$$
(2.33)

Substituting Eqs.(2.31) and (2.32) in to Eq. (2.20) we obtain

$$\langle \vec{V}_{\beta} \rangle = -\left(\frac{\epsilon_{\beta} \xi \lambda_{\beta}}{\mu_{\beta}}\right) \left[\Omega_{\beta} \vec{\nabla} \langle T \rangle - (\rho_{\beta} - \rho_{\gamma}) \vec{g}\right]$$
(2.28)

where

$$\Omega_{\beta} = 2 \, k_{\langle T \rangle} \tag{2.29}$$

2.5.6 Volumetric Constraint

The volume fractions of σ , β and γ phases are defined as:

$$\epsilon_{\sigma} = \frac{V_{\sigma}}{V}, \qquad \epsilon_{\beta} = \frac{V_{\beta}}{V}, \qquad \epsilon_{\gamma} = \frac{V_{\gamma}}{V}$$
(2.30)

Since the sum of the individual volumes occupied by each species must equal the total volume V, then the sum of the individual volume fractions is one.

$$\epsilon_{\sigma} + \epsilon_{\beta} + \epsilon_{\gamma} = 1 \tag{2.31}$$

In our model it is assumed that the pore volume (voids) are always filled with either liquid, gas or a combination. Therefore we can state that the sum of the fluid volume fractions must equal the porosity φ of the studied porous body. Using this assumption we can rewrite Eq. (2.31) as

$$\epsilon_{\sigma} + \varphi = 1 \tag{2.32}$$

2.5.7 γ-phase Diffusion Equation

In their work The Drying of Solids, Comings and Sherwood state:

"At certain stages in the drying of many solids the water moves as a liquid part way to the solid surface and then diffuses as water vapor through the air-filled openings in the porous solid near the surface." [17]

There are two important diffusional resistances that we will consider in our model. First, the resistance to liquid motion in the interior of the solid. This one, mainly due to capillary forces, has been thoroughly considered in the formulation of the equation of motion. The second one is the resistance to diffusion of water vapor through the air-filled pores in the surface of the coffee bean. Using Eq. (2.21)

we can formulate an equation of continuity for either dry air or water vapor species. This equation will be independent from the continuity of gas phase, since it will include the inter-diffusion of gas species. This diffusive term is obtained by substituting Fick's Law in the discontinuity terms that appear from averaging the intrinsic phase density of vapor species. The diffusion of vapor into the gas phase is then given by

$$\frac{\partial \left(\epsilon_{\gamma} \langle \rho_{1} \rangle^{\gamma}\right)}{\partial t} + \nabla \cdot \left(\langle \rho_{1} \rangle^{\gamma} \langle \vec{V}_{\gamma} \rangle\right) - \langle \dot{m} \rangle = \nabla \cdot \left[\langle \rho_{\gamma} \rangle^{\gamma} D_{eff} \nabla \left(\frac{\langle \rho_{1} \rangle^{\gamma}}{\langle \rho_{\gamma} \rangle^{\gamma}}\right)\right]$$
(2.33)

2.6 Porous Media Effective Parameters

Most of the complexities that came up from the averaging of non-linear terms (dispersion vectors) are reduced by introducing effective parameters. However, there is a general drawback; the accuracy of our model depends substantially in the experimental work done to determine these coefficients. In *A Theory of Drying in Porous Media*, Whitaker [22] wrote: "Once again we have swept all of our difficulties into one parameter, the total effective diffusivity, and experimental determination of this parameter, even for an isotropic media, will be a very difficult matter". The following sub-sections present the correlations or modeling used to determine these parameters as well as other important properties.

2.6.1 Spatial Density

To calculate the total energy change of our system we need to define the spatial density. This density represents the total mass per unit volume and is given by Eq.(2.31).

$$\langle \rho \rangle = \epsilon_{\sigma} \langle \rho_{\sigma} \rangle^{\sigma} + \epsilon_{\beta} \langle \rho_{\beta} \rangle^{\beta} + \epsilon_{\gamma} \sum_{i=1}^{N} \langle \rho_{i} \rangle^{\gamma}$$
(2.34)

To calculate the solid phase density we will employ the following expressions, experimentally deducted by Perez-Alegria and Ciro-Velásquez [2001].

$$\rho_{\sigma-bulk} = 5.9993 M_{(\%,b.)} + 282.40 \qquad (r^2 = 0.9742)$$

$$\rho_{\sigma-kernel} = 5.6561 M_{(\%,b.)} + 647.23 \qquad (r^2 = 0.9832) \qquad (2.35)$$

$$0.04 \le M_{(w,b.)} \le 0.56$$

It is necessary to clarify that the bulk density refers to the mass per unit of total volume of parchment coffee. Thus, it includes the void volume. On the other hand, the kernel density is the phase density of coffee mass; without including the void space in the calculation. Both will be used to determine the porosity, since it is define as the void volume per unit of total volume .

$$\varphi = 1 - \frac{\rho_{\sigma-bulk}}{\rho_{\sigma-kernel}} \tag{2.36}$$

While the coffee mass density will be evaluated as a function of the wet-base moisture content, the fluid phases (β and γ) densities will be correlated to the volume averaged temperature. The water vapor density (ρ_1) will be determine using Eq. (2.37) developed by Tortike [1989].

$$\rho_{1} = -93.7072 + 0.833941 T - 0.00320809 T^{2} + 6.57652 x 10^{-6} T^{3} - 6.93747 x 10^{-9} T^{4} + 2.97203 x 10^{-12} T^{5}$$
(2.36)

In like manner, the dry air and liquid water densities will be obtained from the correlations presented in Eqs. (2.37) and (2.38).

$$\rho_2 = 0.001293/(1+0.00367T) \tag{2.37}$$

$$\rho_{\beta} = 1.30753 \times 10^{-8} T^3 - 5.44149 \times 10^{-6} T^2 - 6.00025 \times 10^{-6} T + 1.00039$$
(2.38)

As was previously stated (section 2.5.2), for the gas phase species, the intrinsic phase average density is different from the density evaluated at the averaged phase temperature. The main reason for this is that the gas phase is compressible and the density is a function of both temperature and phase volume fraction. This is more evident in the funicular state (early stage) when the porous media is saturated and the volume occupied by the gas phase is minimum. At the latter stage (pendular state) of the process, Eqs. (2.36) and (2.37) are a good estimate of the gas phase species densities. After the water saturation level decreases, due to the initial vaporization stage, the gas phase occupies basically all the void space between coffee beans. At this point we still have to determine the distribution of the gas species (water vapor and dry air) in the γ phase. However, we can state that at this stage the intrinsic average phase densities are only a function of temperature. This deduction is based on the assumption that the γ phase is ideal in the thermodynamic sense. In an ideal gas, the species do not interact with each other and thus we say that they occupy the same volume.

2.6.2 Heat Capacity

The local resistance of our system (solid-liquid-gas) to increase or decrease its temperature could be represented by its equivalent heat capacity. This will be calculated via the use of a mass fraction weighted average of the different specific heats, as shown on Eq. (2.39).

$$C_{p} = \frac{\epsilon_{\sigma} \langle \rho_{\sigma} \rangle^{\sigma} (c_{p})_{\sigma} + \epsilon_{\beta} \langle \rho_{\beta} \rangle^{\beta} (c_{p})_{\beta} + \epsilon_{\gamma} \sum_{i=1}^{N} \langle \rho_{i} \rangle^{\gamma} (c_{p})_{i}}{\langle \rho \rangle}$$
(2.39)

This weighted average allows us to combine the contribution of each species to the total energy of the system. With this coefficient we couple the mass volume fractions to the total energy equation. To obtain the specific heat of the parchment coffee mass we will employ Eq. (2.40), published by Perez-Alegria and Ciro-Velásquez [30].

$$(c_p)_{\sigma} = 0.0535 M_{(\%,b)} + 1.6552$$
 (2.40)

The specific heat of liquid water, dry air and water vapor will be determined using the correlated data presented by Incropera and DeWitt [36].

2.6.3 Effective Thermal Conductivity

In the formulation done by Whitaker [22] the difficulty represented by the dispersion vector terms is handled by incorporating it into the effective thermal conductivity tensor. In a case were the conductivity of the solid phase is expected to be much more significant, as ours, the dispersion vector can be considered to be negligible [37]. That being the case, the effective thermal conductivity reduces to Eq. (2.41).

$$k_{eff} = \epsilon_{\sigma} k_{\sigma} + \epsilon_{\beta} k_{\beta} + \epsilon_{\gamma} k_{\gamma}$$
(2.41)

The bulk thermal conductivity will be determine using the correlation developed by Perez-Alegria and Ciro-Velásquez [2001].

$$k = 0.00002 M_{(\%w.b.)} + 0.0087$$
 (2.42)

2.6.4 Total Effective Diffusivity

As mentioned at the beginning of this section, all the difficulties of modeling the gas phase diffusion phenomena are incorporated into the total effective diffusivity. This coefficient represent the proportionality between the molar flux of water vapor through the porous media and the gradient of water vapor concentration. The higher this value, the faster the water vapor will diffuse into the gas phase. For a porous media, this diffusion process is highly dependent of the topology of the pores. This dependence is usually accumulated in the so-called tortuosity vector. However, we can determine the effective diffusivity without characterizing the pore structure of the coffee bean by experimentally correlating it using the Arrhenius equation (Eq. 1.23). This relation assumes that on the average this coefficient depends only on the temperature. Assuming that the shrinkage effects are negligible and that diffusion of water vapor occurs strictly at the surface of the coffee beans, Corrêa [31] developed the following expression for the effective diffusivity coefficient.

$$D_{eff} = 2.041 \times 10^{-6} \exp\left(\frac{-22.619}{RT}\right)$$
(2.43)

Where *R* is the universal gas constant presented below.

$$R = 0.008314 \, kJ/mol - K \tag{2.44}$$

2.6.5 Single Coffee Bean Permeability

One of the most important parameters involving any flow characterized by Darcy's law is the permeability of the porous body. Permeability could be defined as the mean effective area normal to a fluid flow passing through a porous material. Clearly, the permeability tensor is a direct function of the topology of the porous body. Therefore, experimentation is required to determine its value. This is a big limitation for our study, since there is no permeability data for parchment coffee (*C.Arabica*) available at this moment. To estimate the permeability of a single coffee bean, we will employ the method developed by Marshall [38] . In his work, he published a mathematical expression relating the permeability and the pore size distribution of an isotropic material. The assumptions of this methodology are the following:

- The material is isotropic or its pore space is randomly distributed.
- There are no lengthy conducting channels.
- The rate of flow is controlled by the cross-sectional area of the necks connecting the pores and obeys Darcy's law.
- The pore channel is assumed to be straight. This assumption is based on the work done by Slichter [39], where he demonstrates that the errors of this approximation are mutually compensating.

This assumptions seem reasonable with the exception of the isotropy of our porous material. To assume that a coffee bean (*C.Arabica*) is an isotropic porous media we need some experimental evidence. In his work concerning the micro-structure of *C.Arabica*, Pittia concludes:

"The methodological approach to the evaluation of the porosity in green beans under study

evidenced a limited presence of voids or pores differently distributed between the internal and external volumes " - [40]

Based on the evidence provided by Pittia [40] we decided to assume that the coffee bean studied herein is an isotropic porous media. Using this assumptions, we implemented Marshall's methodology. The concept behind his method is that the linear stream-line velocity governed by Darcy's law (Eq. 2.45) must be equal to Poiseuille's solution (Eq. 2.46) for mean velocity inside a narrow circular tube. Comparing this two expressions and relating the mean equivalent pore cross-section radius (R_e) to the pore size distribution he developed Eq. (2.47). This allows us to estimate the permeability characteristic of a single coffee bean.

$$u = -\frac{\lambda}{\mu} \frac{dP}{ds} \tag{2.45}$$

$$u_{mean} = \frac{-\varphi R_e^2}{8\mu} \frac{dP}{ds}$$
(2.46)

$$k = \frac{1}{8}\varphi^2 n^{-2} \left(r_1^2 + 2r_2^2 + 5r_3^2 + 7r_4^2 + \dots + (2n-1)r_n^2 \right)$$
(2.47)

Where

$$r_1 > r_2 > r_3 > r_4 > \dots > r_n$$
 (2.48)

Now, to evaluate Eq. 2.47 we need to know the porosity φ and the pore radius (r_i) distribution. Pittia [40] reported that the pore size distribution is dominated by macropores in a range between 10 to 70 µm. As it can be seen, Eq. 2.47 does not depends on the frequency of a pore radius, since it is assumed to be randomly distributed. This means, using the law of large numbers, that as we increase the number of terms in the distribution (n), the sum of terms at the right side of Eq. 2.47 becomes closer to the mean equivalent radius (R_e). To do our permeability estimate, a random distribution of 500 terms between 10 and 70 µm was used. The distribution generated in this step is shown in Figs. 2.6.1 and 2.6.2.



Figure 2.6.1: Random Pore Size Distribution



Figure 2.6.2: Pore Size Distribution Histogram

After generating the pore size distribution, the different radii were sorted in descending order to satisfy Eq. (2.48). The next step in the methodology was to select the proper value of porosity. We already discussed, at Eq. (2.36), how to determine the macro-porosity of our system. Now, we need to distinguish between that porosity and the porosity of a single coffee bean. The former will be identified in this study as the micro-porosity. In his work, Pittia [40] presented the following data for *C.Arabica* green bean.

Porosity (φ)					
Coffee Bean	External 1	External 2	Internal	Average	Uncertainty
Green	0.041	0.041	0.064	0.049	± 0.004

Table 2.6.1: Porosity of Green Coffee Beans in 2 External and Internal Regions [40]

Although this data is for green coffee beans, it could be used under the assumption that shrinkage effects are negligible. For the estimate of coffee bean permeability we used an average porosity value of 0.049. Substituting the previously determined pore size distribution and this average porosity value into Eq. (2.47) we obtained a value of 1.444E-7 cm² for the permeability of a single coffee bean.

2.6.6 Bulk Permeability

In section 2.6.5 we estimated the permeability of a single coffee bean using the pore size distribution and porosity of a single grain. This permeability is indeed the effective area for the motion of liquid water in our porous media as could be seen in Eq. (2.49). It is also the effective area for the motion of gas in the portion of our control volume occupied by the solid .

$$k_{\beta} = k_{bean} = 1.44 \times 10^{-7} \ cm^2 \tag{2.49}$$

To calculate the total permeability of gas phase, we must understand that the air will have a different

permeability depending if it is located in the region occupied by the solid phase or in the void space between grains (macro-pore). Our approach to determine a characteristic permeability for the γ phase was to formulate a volume weighted average between the micro-scale and macro-scale permeabilities. In the void space (φ) the permeability of the air will be the still undetermined coffee bed permeability (k_{bed}) and everywhere else (1- φ) the characteristic permeability will be assumed to be the the microscale permeability (k_{bean}). The formulation of this bulk permeability is seen in Eq. (2.50).

$$K = \varphi k_{bed} + (1 - \varphi) k_{bean}$$
(2.50)

Even though we are assuming the micro-scale permeability to be constant (due to negligible shrinkage effects), the bulk permeability will vary as the bulk porosity varies. Therefore, the permeability of the gas phase will be a function of porosity as shown in Eq. (2.51).

$$k_{\gamma} = K = f(\varphi) \tag{2.51}$$

The remaining difficulty is to estimate the bed permeability (k_{bed}). This could be done using Eq. (2.47), as long as we know the macro-pore size distribution. To determine the macro-pore size distribution we will assume that our control volume consists of the interaction of perfectly spherical beans of equivalent diameter D_e . In the future, the concept of sphericity could be incorporated into this formulation, but at the moment we will make this radical assumption. Based on observation, it was decided to represent our control volume using an analogy to cubic crystal structures as shown in Fig. 2.6.4.



Figure 2.6.3: Porous Media Control Volume Used for Macro-Permeability Estimate

To generate the macro-pore size distribution we assumed that the pore diameter varies from a less packed configuration to a close-packed one. Therefore, the minimum pore radius is equivalent to the space between atoms (λ) in an FCC configuration as formulated in Eq. (2.52) and the maximum pore radius is equivalent to the space between atoms in a BCC configuration (Eq. 2.53).

$$\lambda_{\min} = 2R \tag{2.52}$$

$$\lambda_{max} = 2\left(\sqrt{(3)} + 1\right)R \tag{2.53}$$

Where,

$$R = \frac{D_e}{2} \tag{2.54}$$

From the data published by Perez-Alegria [2001] it can be determined that the mean equivalent diameter for parchment coffee (*C.Arabica*) is 7.87E-3 m. With this equivalent diameter, and using Eqs. (2.52) and (2.53), we determined that the macro-pore distribution is in a range between 7.87 to 21.4 mm. Subsequently, we generate a random distribution of 70 values inside the calculated range as illustrated in Figs. 2.6.5 and 2.6.6.



Figure 2.6.4: Random Macro-Pore Size Distribution



Figure 2.6.5: Macro-Pore Distribution Histogram

In figure 2.6.6 we can observe that the probability of our random distribution is uniform. This is important to state that our distribution was really random. All the events (possible radii) should have the same probability of occurrence. Using the macro-pore distribution obtained it is possible to calculate the coffee bed permeability by employing Eq. (2.47). Evaluating our results for coffee bed permeability and single bean permeability in Eq. (2.50) we obtained the following relationship between bulk permeability and wet base moisture content.



Figure 2.6.6: Bulk Permeability of Parchment Coffee (C.Arabica)

It is important to remember that the permeability of air will be the same as the bulk permeability. Therefore, Figure 2.6.7 represents a prediction of the permeability of air in parchment coffee throughout its drying process. It is interesting that the permeability of air in our medium is in the same order of its permeability in well-sorted gravel (10E-3), given that they physically look alike. The results shown in this section were implemented in the modeling of the dehydration process of parchment coffee (*C.Arabica*) presented in our study. At the moment this study is written, no data or estimate of the permeability of air (and water) in coffee mass has been published.

2.6.7 Topological Parameter (ξ)

As we discussed in Section 2.5.5, the parameter ξ in the liquid motion equation (Eq. 2.29), is a function inversely proportional to the number of phase discontinuities in β phase. It was explained that at the beginning of the dehydration process the phase is continuous and therefore the number of discontinuities is 1. It was also discussed that as the coffee becomes dry, the number of discontinuities goes to infinite, leading our topological parameter to be 0. Based on the understanding of the process, it was proposed to model this parameter as a function of the moisture content. To physically represent this

parameter in terms of transport quantities, we represented it as the ratio between the actual liquid volume fraction and its initial value. This expression is shown in Eq. (2.55).

$$\xi = \frac{\epsilon_{\beta}}{\{\epsilon_{\beta}\}_{t=0}}$$
(2.55)

2.7 Pressure Calculations

One of the drawbacks of this methodology is that the pressure field must be either known or determined using laminar boundary layer theory. In our work we will constrain the vapor phase pressure gradient to be constant and we will impose boundary conditions based on the inlet and outlet pressure determined experimentally.

Pressure Constraint
$$\nabla p_1 = constant$$
 (2.56)

Using the relative humidity data obtained in our experiment, we can determine the vapor pressure at both the inlet and the outlet of our system by using Eq. (2.57). The vapor saturation pressure will be evaluated using the thermophysical properties data presented by Moran and Shapiro [41].

$$p_1 = RH \ p_{sat} \tag{2.57}$$

2.8 Mathematical Model Summary

The mathematical model presented here aims to predict the temperature and moisture content dynamics during the studied process. There are a total of 12 unknown quantities to solve in this system of coupled phenomena.

12 unknowns \rightarrow $\langle T \rangle, \langle \vec{V}_{\beta} \rangle, \langle \vec{V}_{\gamma} \rangle, \epsilon_{\beta}, \epsilon_{\gamma}, \langle \dot{m} \rangle,$ $\langle p_{\gamma} \rangle^{\gamma}, \langle p_{1} \rangle^{\gamma}, \langle p_{2} \rangle^{\gamma}, \langle \rho_{\gamma} \rangle^{\gamma}, \langle \rho_{1} \rangle^{\gamma}, \langle \rho_{2} \rangle^{\gamma},$ The formulated system of equations consist of the following 6 transport equations

- Total thermal energy (Section 2.5.1)
- γ phase continuity (Section 2.5.2)
- β phase continuity (Section 2.5.3)
- γ phase motion (Section 2.5.4)
- β phase motion (Section 2.5.5)
- Vapor diffusion equation (Section 2.5.7)

In addition to this equation we have two other constraints related to the volumetric fractions (Section 2.5.6) and the pressure field (Section 2.7). That leaves us with 8 equations and 12 unknown quantities. At this point, 4 additional relations are required to have a well posed problem from an algebraic point of view. The first two relationship are based on the assumption that the gas phase is ideal in a thermodynamic sense. Using Eqs. (2.58) and (2.59) we can relate the pressure of the gas species to the temperature using the ideal gas law.

$$\langle p_1 \rangle^{\gamma} = \langle \rho_1 \rangle^{\gamma} R_1 \langle T \rangle$$
 (2.58)

$$\langle p_2 \rangle^{\gamma} = \langle \rho_2 \rangle^{\gamma} R_2 \langle T \rangle$$
 (2.59)

Where R_1 and R_2 are obtained by dividing the universal gas constant by the molecular weight of each species. Since both the dry air and the water vapor are assumed to be constant, they are supposed to share the same volume. Therefore we can state that the intrinsic phase average density of the γ phase is the sum of the individual species intrinsic phase average density.

$$\langle \rho_{\gamma} \rangle^{\gamma} = \langle \rho_{1} \rangle^{\gamma} + \langle \rho_{2} \rangle^{\gamma} \tag{2.60}$$

Also we can state that the total pressure is equal to the sum of the partial pressures, based on Dalton's law.

$$\langle p_{\gamma} \rangle^{\gamma} = \langle p_{1} \rangle^{\gamma} + \langle p_{2} \rangle^{\gamma}$$
(2.61)

With this last equation we completed a total of 12 expressions to relate the 12 unknown transport quantities. This only means that it is possible to algebraically solve this system of equations. As it could be seen throughout this chapter, the equations that describe our phenomena are non-linear and highly coupled. Consequently, numerical methods are required to find the solution of this problem. However, depending on the selection of boundary conditions, the solution could be either good, make no sense or does not exist. The next chapter of this study is dedicated to the selection and implementation of a numerical method to solve this coupled system of equations.

3 Numerical Solution

In chapter 2 we presented the mathematical model describing the dehydration process of our porous body. It is clear that this system of equations, as presented, does not have any analytical solution. Consequently, a numerical method must be implemented to find a solution. In this chapter, we will present the employment of the finite volume method in order to solve these equations. This set of equations is coupled, mathematically and phenomenologically. It means that to properly solve the equations we will need to understand the numerical weight of the different phenomena interacting in this process. To refine the knowledge of the phenomena presented in the former chapter, a dimensionless analysis of our system of equations is presented herein. Using the physical deductions obtained from our analysis, its possible to develop a solution strategy.

3.1 Physical Domain

The equations presented in our study are general enough to include the possibility of implementing this model to various porous media and diverse machinery. However, the model will be calibrated using experimental data from an unique porous body dehydrated in an unique device. The studied volume consists of a parchment coffee bed with a total diameter of 0.646 meters (25.5 in) and a height of 0.235 meters (9.25 in). A schematic representation is presented below (Figure 3.1.1).



Figure 3.1.1: Schematic Representation of the Porous Media

3.1.1 Mesh Generation

To algebraically solve equations involving differentials (derivatives, gradients, etc.) we must first transform a continuous space (with infinite subdivisions) into a discrete space with finite subdivisions. To model the concerning phenomena we will solve the coupled system of equations proposed in chapter 2 over a quasi-three dimensional space. This will be done by assuming cylindrical symmetry around z-axis. It is a valid assumption when the transport quantities distributions are uniform revolving z-axis. In our case, that is a reasonable statement since the drying equipment has an internal agitator that mixes the coffee beans step-wise. With this simplification the studied physical domain reduces to a 2-D space with a width equal to the radius of the rotary drum dryer and height equal to the height of the coffee bed. This domain is shown on Figure 3.1.2.



Figure 3.1.2: Quasi-Three Dimensional Discrete Domain

$$V_{cell} = dr \, dz \tag{3.1}$$

The volume (V) contained in this space will be divided into cells of volume per unit depth V_{cell} which is represented by Eq. (3.1). Although the visual representation is a rectangular space, we should not forget that this is just a simplification from a cylindrical coordinates system. Even though the volume per unit depth of each cell is the same, the actual volume represented by each cell becomes greater as we move far from the symmetry axis. Therefore, the discretization of the volume averaged transport equations shall consider that fact. Another important subject we must pay attention to is the selection of a proper mesh resolution. When a continuous space is transformed into discrete volumes, each generated cell must be small enough to properly transmit information to neighbor cells. In the following section (3.1.2) a mesh resolution sensibility analysis is presented.

3.1.2 Mesh Resolution Sensibility Analysis

To select a proper mesh resolution for our numerical method a resolution sensibility analysis is required. The purpose of this is to prove that the results obtained from our numerical method are independent from the mesh resolution selected. The sensibility to changes in the mesh resolution is an unique characteristic of each model. Therefore we need first to be able to solve our set of equations to perform a sensibility analysis. The selection and implementation of numerical schemes to solve these equations will be discussed in the next few sections. However, this section will make reference to the numerical methods included in following sections and present a mesh resolution sensibility analysis based on our results.

The sensibility analysis was performed using three different mesh resolutions of 25x25, 50x50 and 80x80 cells. Using a time step of 1 minute, the coupled system of equations was solved given a known air inlet temperature of 43.8 °C and a given air inlet speed of 1.8E-03 m/s. The results for the temperature distribution after 1 hour of drying of these three cases is presented in Figs. (3.1.3), (3.1.4) and (3.1.5).



Figure 3.1.3: Temperature Distribution in Coffee Mass Bed at t=1 hr (25x25 Cells)



Figure 3.1.4: Temperature Distribution in Coffee Mass Bed at t=1 hr (50x50 Cells)



Figure 3.1.5: Temperature Distribution in Coffee Mass Bed at t=1 hr (80x80 Cells)

From the images above we can state that the temperature profile does not vary significantly as we move from a less dense mesh to a more dense one. In spite of that, a qualitative comparison is not enough to determine the magnitude of the variation of the temperature due to changes in the mesh resolution. For a more accurate analysis, lets use Fig. (3.1.6) in which the temperature is monitored for 10 minutes using 6 different mesh resolutions. The temperature plotted here is taken from the cell equivalent to position r = 0.16 m and z= 0.118 m. From this image it is clear that the temperature increases slightly as the resolution increases. This variation becomes less apparent as we reach the highest resolution plotted. A mesh resolution of 50x50 nodes was selected, in order to generate a mesh for which the temperature is independent of the cell size. This was determined based on the effects of cell size in the temperature, since the temperature is the transport quantity that experiments more variations throughout the dehydration process. It can be argued that the moisture content experiments

even more variation due to the nature of the drying process. However, there are two reasons to not use the moisture content (either liquid volume fraction or wet base average) as our critical quantity in this analysis. First, as illustrated in Fig. (2.1), the early stage of the dehydration process is characterized by a constant drying rate. That means that the moisture distribution is almost uniform and the effects of mesh resolution are minimum. Second, at the latter stage the drying rate decreases dramatically and the variations of the moisture content from one time step to another are very small.



Figure 3.1.6: Sensibility of the Coffee Mass Temperature to Mesh Resolution

3.1.3 Boundary Conditions

The selection and implementation of boundary conditions is critical to properly model any phenomena and a dehydration process is not the exception. It has been reported that for different boundary conditions the solution will represent a different flow, temperature and moisture distribution [42]. In our case, due to the non-linearity of the equations we need to consider 2 criteria when selecting the appropriate boundary conditions: (1) *the boundary conditions should represent at its best*
the real conditions of the physical phenomenon under study and (2) they should be strategically imposed to enhance the convergence properties of our numerical method.

The boundary conditions for the temperature field are presented in Eqs (3.2)-(3.5). The temperature at the bottom of the coffee bed was assumed to be equal to the air inlet temperature, thus imposing a wall condition on the bottom boundary (Eq. 3.2). This supply air temperature (T_{SA}) will be an input function based on the configuration of the drying equipment used. At time t = 0 the temperature at every point is equal to the initial temperature $T_0 = 23$ °C with the exception of the bottom surface as shown on Eq. (3.3). In Eq. (3.4) it is stated that the heat flux is zero at r = 0 and r = R. At the center of the drum dryer this is assumed due to axis-symmetry and at the circumference of the drum because the equipment used to take the experimental data was insulated on the outer surface.

$$\langle T \rangle_{z=0,t>0} = T_{SA} \tag{3.2}$$

$$\langle T \rangle_{z \neq 0, t=0} = T_0, \ \langle T \rangle_{z=0, t=0} = T_{SA}$$
 (3.3)

$$\left(\frac{\partial \langle T \rangle}{\partial r}\right)_{r=0,t>0} = 0, \ \left(\frac{\partial \langle T \rangle}{\partial r}\right)_{r=R,t>0} = 0$$
(3.4)

In the former expressions, the boundary conditions for the temperature field has been presented excluding the air outlet (z = H). To select a boundary condition for this surface we will quote the words of H. K. Versteeg and W. Malalasekera [43]: "If the location of the outlet is selected far away from geometrical disturbances the flow often reaches a fully developed state where no change occurs in the flow direction". In our case, this could be assumed since our flow is within Darcy regime. Furthermore, the resistance to flow represented by the parchment coffee bed makes the effects of inlet flow negligible at the outlet. The gradients of all transport quantities (excluding clearly the pressure) could be set to zero at the outlet surface without incurring in significant error. In subsequent discussion, this will be referred to as the zero gradient outlet assumption. For the temperature field this can be written as

$$\left(\frac{\partial \langle T \rangle}{\partial z}\right)_{z=H, t \ge 0} = 0 \tag{3.5}$$

The boundary conditions for the motion of liquid phase is presented in Eqs. (3.6)-(3.7). The velocity of the liquid phase is set to zero at the walls of the drum dryer due to the no-slip condition. Likewise, the velocity at the inlet (z = 0) is set to zero, because the volume fraction of the liquid phase is assumed to be zero at the entrance; only gas occupies the entrance of our system. To impose the boundary condition at the exit surface (z = H) we will make reference to the zero gradient outlet assumption as shown in Eq. (3.8).

$$\langle \vec{V}_{\beta} \rangle_{r=0, t \ge 0} = 0, \ \langle \vec{V}_{\beta} \rangle_{r=R, t \ge 0} = 0$$
(3.6)

$$\langle \vec{V}_{\beta} \rangle_{z=0, t \ge 0} = 0 \tag{3.7}$$

$$\left(\frac{\partial \langle \vec{V}_{\beta} \rangle}{\partial z}\right)_{z=H,\,t>0} = 0 \tag{3.8}$$

Similar to the boundary conditions for the motion of liquid phase, the motion of gas phase at the walls of the drum dryer is set to zero (Eq. (3.9)). However, at the air inlet, we assume that flow exists only in the z-direction and that it is equal to the volumetric flow provided by the fan per unit area. This flow is corrected by a factor $C_{entrance}$ (equal to 0.78 in our case) due to an obstruction at the inlet caused by a sheet metal grid. For the velocity at the outlet we assumed the velocity gradients in z-direction to be zero (zero gradient assumption).

$$\langle \vec{V}_{\gamma} \rangle_{r=0, t \ge 0} = 0, \ \langle \vec{V}_{\gamma} \rangle_{r=R, t \ge 0} = 0$$
(3.9)

$$\langle \vec{V}_{\gamma} \rangle_{t \ge 0, z=0} = 0\,\hat{i} + 0\,\hat{j} + C_{entrance} \frac{Q_{fan}}{A_{SA}}\hat{k}$$
(3.10)

$$\left(\frac{\partial \langle \vec{V}_{y} \rangle}{\partial z}\right)_{z=H,t>0} = 0$$
(3.11)

To determine the boundary conditions for the phases volume fractions we must make reference to the liquid phase continuity equation presented at Eq. (2.24). If we wanted to integrate this equation to obtain the volume fraction at any time we would just need an initial condition. To determine the initial value of the volume fractions its necessary to introduce an expression relating the wet based moisture content (ψ) to the volume fraction of β -phase. Recalling that the volume fraction is the ratio of the volume occupied by a phase to the total volume we can write Eq. (3.12). Using Eq. (3.13) and knowing from our experimental data the initial value of the moisture content, we can find the initial condition for the volume fraction of water.

$$\psi_{t=0} = \left\{ \frac{\rho_{\beta} V_{\beta}}{\rho_{\beta} V_{\beta} + \rho_{\sigma} V_{\sigma}} \right\}_{t=0} = \left\{ \frac{\rho_{\beta} \epsilon_{\beta}}{\rho_{\beta} \epsilon_{\beta} + \rho_{\sigma}} \right\}_{t=0}$$
(3.12)

$$\{\epsilon_{\beta}\}_{t=0} = \left[\frac{\psi \rho_{\sigma}}{(1-\psi)\rho_{\beta}}\right]_{t=0}$$
(3.13)

If we combine Eqs. (2.31) and (3.13) we can relate the initial volume fraction of gas phase to the initial volume fraction of liquid phase as shown in Eqs. (3.14) and (3.15)

$$\epsilon_{\gamma,t=0} = 1 - \epsilon_{\sigma,t=0} - \epsilon_{\beta,t=0}$$
(3.14)

$$\epsilon_{\gamma, t=0} = 1 - (1 - \varphi)_{t=0} - \left[\frac{\psi \rho_{\sigma}}{(1 - \psi) \rho_{\beta}} \right]_{t=0}$$
(3.15)

These boundary conditions, Eqs. (3.2) to (3.15), complete the set of conditions entailed to have an

algebraically well-posed system of partial differential equations (PDE). Other transport quantities such as the vaporization mass flow rate, the gas pressure and the phase densities do not, mathematically, require any boundary condition since they are not involved in any differentiation process and can be deduced from other transport quantities. The term "mathematically" is employed here since these quantities may require some numerical constraints to ensure compliance with fundamental laws, such as the conservation of mass principle.

The first numerical constraint we will imposed is the conservation of mass at the outlet of the system. Even when this principle is implicit in the formulation of the volume averaged continuity equations we will verify if this is being satisfied. The reason is that such a coupled system of PDE needs to be solved iteratively. At the intermediate iterative steps (when the equations are not yet simultaneously satisfied) failing to comply with the conservative principle could cause our system to diverge. The mass flow entering our system should be equal to the total mass exiting minus the mass of water evaporated in the studied domain. It can be expressed as

$$\dot{m}_{inlet} = \dot{m}_{outlet} - \dot{m}_{evap} \tag{3.16}$$

The second numerical constraint is that the initial mass flow rate is not exactly zero. A constant value of initial vaporization rate will be assumed to avoid zero division at the beginning of the iterative solution method. This value should be small to avoid any significant deviation from the solution.

$$\langle \dot{m} \rangle_{z>0, t=0} = 1 \times 10^{-4} \frac{kg}{m^3 \cdot s}$$
 (3.17)

With Eq. (3.17) we finish the list of conditions that will be numerically imposed to our system of equations. More detail on the implementation and consequences of these conditions will be presented later in this study.

3.2 Dimensionless Analysis of Transport Equations

One of the challenges of modeling a multistage process such as the one studied herein is understanding the phenomena behind the process and how their contribution to the process in general may be considerable at times and at times may not. This understanding is necessary to reduce the computational cost of our model. It is very common that one of the terms relevant in one part of the process is almost negligible in other part of the same process. Ignoring some terms, when its reasonable, could reduce our computational cost without adding significant error to our calculations. On the other hand, keeping such a small term could be a source of error by inducing numerical noise. To understand the contribution of the different phenomena responsible for the dehydration of our porous media we will use the well-known dimensional analysis [44].

3.2.1 Dimensionless Parameters

The dimensional analysis is done by substituting our dimensioned variables by an equivalent expression relating this dimensioned variables to their dimensionless form via the use of a reference value. In Eqs. (3.18) to (3.21) we introduce the dimensionless variables that are required in the dimensional analysis of our mathematical model. The dimensionless length is presented in Eq. (3.18) as the ratio of any dimensioned length to the characteristic length of our porous media. Since, the scope of this study is to model the dehydration process at the level of a single bean and not at the micro-scale, the characteristic length used will be the average coffee grain diameter. In the case of the dimensionless velocity, presented in Eq. (3.19), it will be represented as the ratio of the velocity to the air inlet speed. The dimensionless time, will be equal to the ratio of the time to the characteristic time of the process. This characteristic time will be calculated dividing the characteristic length by the air inlet velocity. To calculate the dimensionless temperature we will select our reference temperature as the maximum temperature difference in our system as shown in Eq. (3.21). The drawback of choosing this temperature is that the value of the dimensionless temperature could be sometimes higher than 1. This is done, instead of using a fixed position temperature, due to our need of using a constant reference value. The dimensionless densities will be evaluated in reference to the air inlet density as shown in Eq. (3.22).

$$\hat{l} = \frac{l_i}{l_c} \tag{3.18}$$

$$\hat{V} = \frac{V}{U_{\infty}} \tag{3.19}$$

$$\hat{t} = \frac{t}{t_c} \tag{3.20}$$

$$\hat{T} = \frac{T}{\Delta T_{max}} \tag{3.21}$$

$$\hat{\rho} = \frac{\rho}{\rho_{\infty}} \tag{3.22}$$

3.2.2 Dimensionless Numbers

Substituting the dimensioned quantities by expressing them using Eqs. (3.19) to (3.22) will force the apparition of some dimensionless numbers common in the field of heat and mass transfer. Sometimes the terms involving these numbers will be obvious, but sometimes it will require some algebraic manipulation of the equations. These dimensionless numbers represent the ratio between two specific forces or phenomena and their magnitude could be interpreted as the dominance of one phenomena over the other. In our dimensional analysis we will introduce the following dimensionless numbers:

Reynolds Number

$$Re = \frac{\rho_{\infty}U_{\infty}l_{c}}{\mu_{\infty}} = \frac{\text{inertia force}}{\text{viscous force}}$$
(3.23)

Prandtl Number

$$Pr = \frac{Cp_i \mu_i}{K_i} = \frac{viscous \, dissipation}{thermal \, dissipation}$$
(3.24)

$$Fo = \frac{K_{eff}t_c}{\langle \rho \rangle C_p L_c^2} = \frac{thermal \, diffusion \, rate}{storage \, rate}$$
(3.25)

Capillary Number

$$Ca = \frac{\lambda_i P_c}{l_c U_{\infty} \mu_i} = \frac{capillary \ force}{viscous \ force}$$
(3.26)

Gravity Number

$$Gr = \frac{\lambda_i \rho_i g}{U_{\infty} \mu_i} = \frac{gravity \ force}{viscous \ force}$$
(3.27)

Schmidt Number

$$Sc = \frac{\mu_i}{\langle \rho_1 \rangle^{\gamma} D_{eff}} = \frac{viscous \, diffusion \, rate}{molecular \, diffusion \, rate}$$
(3.28)

3.2.3 Dimensionless Equations

Using Eqs. (3.19) to (3.22) and introducing the dimensionless numbers from Eqs. (3.23) to (3.28) we obtain the dimensionless form of the volume averaged transport equations. These equations will allow us to apply our physical deductions to improve and simplify our model, as well as improving the convergence of our numerical method described in the following sections.

Dimensionless Energy Equation

$$\frac{1}{Fo}\langle\hat{\rho}\rangle\frac{\partial\hat{T}}{\partial\hat{t}}+Re\left[Pr_{\beta}\hat{\rho}_{\beta}\hat{\vec{V}}_{\beta}+Pr_{\gamma}\hat{\rho}_{\gamma}\hat{\vec{V}}_{\gamma}\right]\hat{\nabla}\cdot\hat{T}=\hat{\nabla}^{2}\hat{T}-\frac{\langle\dot{m}\rangle l_{c}^{2}}{K_{eff}}\frac{\Delta h_{vap}}{\Delta T_{max}}$$
(3.29)

In the early stage of the dehydration process, the vaporization (source) terms dominate the change of energy in the system. If we compare the magnitude of the convective terms, which are of the order of Reynolds number (Re is approximately one for Darcy flow), to the local term (time derivative) and the source term we can determine it to be negligible at this stage. The same could be stated referring to the diffusive term. However, one of the lessons learned in the modeling process is that even when the diffusion-conduction term seems negligible, its contribution is vital to transfer the energy from one computational cell to its neighbors. The consequence of neglecting the diffusive term is that the temperature will increase abnormally at the bottom boundary of our domain causing the solution to diverge. Then, for the early stage of our process the dimensionless energy equation could be written as

$$\frac{1}{Fo} \langle \hat{\rho} \rangle \frac{\partial \hat{T}}{\partial \hat{t}} = \hat{\nabla}^2 \hat{T} - \frac{\langle \dot{m} \rangle l_c^2}{K_{eff}} \frac{\Delta h_{vap}}{\Delta T_{max}}$$
(3.30)

Now, in the latter stage the drying rate rapidly decreases and the transport of energy in the porous media will be more accurately represented by convection-diffusion phenomena. This could be written as shown in Eq. (3.31).

$$\frac{1}{Fo}\langle\hat{\rho}\rangle\frac{\partial\hat{T}}{\partial\hat{t}} + Re\left[Pr_{\beta}\hat{\rho}_{\beta}\hat{\vec{V}}_{\beta} + Pr_{\gamma}\hat{\rho}_{\gamma}\hat{\vec{V}}_{\gamma}\right]\cdot\hat{\nabla}\hat{T} = \hat{\nabla}^{2}\hat{T}$$
(3.31)

Dimensionless β -phase Motion Equation

The dimensionless form of the equation of liquid motion is presented on Eq. (3.32). As can be seen the second term on the right side of the expression is described by the gravity number. For the phenomena analyzed in our study the contribution of gravitational forces is negligible. Therefore, Eq. (3.32) could be simplified into Eq. (3.33).

$$\hat{\vec{V}}_{\beta} = Ca_{\beta}[\xi\epsilon_{\beta}] \left\{ \frac{\partial \hat{P}_{\beta}}{\partial\epsilon_{\beta}} \hat{\vec{\nabla}} \epsilon_{\beta} - \frac{\partial \hat{P}_{\beta}}{\partial\hat{T}} \hat{\vec{\nabla}} \hat{T} \right\} - Gr_{\beta}[\xi\epsilon_{\beta}] [\hat{\rho}_{\beta} - \hat{\rho}_{\gamma}]$$
(3.32)

$$\hat{\vec{V}}_{\beta} = Ca_{\beta} \left[\xi \epsilon_{\beta} \right] \left\{ \frac{\partial \hat{P}_{\beta}}{\partial \epsilon_{\beta}} \hat{\vec{\nabla}} \epsilon_{\beta} - \frac{\partial \hat{P}_{\beta}}{\partial \hat{T}} \hat{\vec{\nabla}} \hat{T} \right\}$$
(3.33)

Dimensionless y-phase Motion Equation

The dimensionless form of the equation of gas motion is presented on Eq. (3.34). With the same reasoning used to analyze the motion of β -phase, based on negligible gravitational effects we can write our dimensionless gas phase motion as shown in Eq. (3.35).

$$\vec{V}_{\gamma} = -Ca_{\gamma}\vec{\nabla}(\vec{P}_{\gamma}-1) + Gr_{\gamma}\hat{\rho}_{\gamma}$$
(3.34)

$$\hat{\vec{V}}_{\gamma} = -Ca_{\gamma}\vec{\nabla}(\hat{P}_{\gamma}-1)$$
(3.35)

Dimensionless β -phase Continuity Equation

The dimensionless liquid phase continuity equation is presented in Eq. (3.36). As state before, in the early stage the vaporization flux prevails over the convective fluxes allowing us to simplify it into Eq. (3.37). In the latter stage, the vaporization mass flow rate becomes negligible and the phenomenon becomes convection-diffusion driven yielding Eq. (3.38).

$$\frac{1}{Fo_{\beta}}\frac{\partial\epsilon_{\beta}}{\partial\hat{t}} + Re_{\beta}Pr_{\beta}\hat{\nabla}(\hat{\vec{V}}_{\beta}) + \frac{1}{Fo_{\beta}}\frac{t_{c}}{\rho_{\infty}}\frac{\langle \dot{m} \rangle}{\hat{\rho}_{\beta}} = 0$$
(3.36)

$$\frac{\partial \epsilon_{\beta}}{\partial \hat{t}} + \frac{t_c}{\rho_{\infty}} \frac{\langle \dot{m} \rangle}{\hat{\rho}_{\beta}} = 0$$
(3.37)

$$\frac{1}{Fo_{\beta}}\frac{\partial \epsilon_{\beta}}{\partial \hat{t}} + Re_{\beta}Pr_{\beta}\hat{\nabla}(\hat{\vec{V}}_{\beta}) = 0$$
(3.38)

Dimensionless y-phase Continuity Equation

The dimensionless gas phase continuity equation is presented in Eq. (3.39). Similar to the dimensional analysis of β -phase continuity, in the early stage the convective fluxes could be neglected simplifying Eq. (3.39) into Eq. (3.40). In the latter stage, the vaporization mass flow rate becomes negligible and the mass conservation of gas phase is best represented by Eq. (3.41).

$$\frac{1}{Fo_{\gamma}}\frac{\partial}{\partial\hat{t}}\left(\epsilon_{\gamma}\hat{\rho_{\gamma}}\right) + Re_{\gamma}Pr_{\gamma}\hat{\nabla}\left(\hat{\rho_{\gamma}}\vec{V_{\gamma}}\right) = \frac{1}{Fo_{\gamma}}\frac{t_{c}}{\rho_{\infty}}\langle\dot{m}\rangle$$
(3.39)

$$\frac{\partial}{\partial \hat{t}} \left[\epsilon_{\gamma} \hat{\rho_{\gamma}} \right] = \frac{t_c}{\rho_{\infty}} \langle \dot{m} \rangle \tag{3.40}$$

$$\frac{1}{Fo_{\gamma}}\frac{\partial}{\partial\hat{t}}\left(\epsilon_{\gamma}\hat{\rho}_{\gamma}\right) + Re_{\gamma}Pr_{\gamma}\hat{\nabla}\left(\hat{\rho}_{\gamma}\hat{\vec{V}}_{\gamma}\right) = 0$$
(3.41)

Dimensionless Vapor Diffusion Equation

A dimensionless form of the vapor diffusion equation is presented on Eq. (3.42). From our physical understanding we can simplify and adjust this equation for the two main stages of the drying process. At the initial stage, vaporization prevails over convective transport. Also, the mass diffusion is meaningless since the porous media is saturated and no concentration gradient exists. Eliminating both the convection and mass diffusion terms we obtain Eq. (3.43). In the later stage the vaporization rate becomes negligible and convective-diffusive transport takes place as shown in Eq. (3.44).

$$\frac{1}{Fo_{\gamma}}\frac{\partial}{\partial\hat{t}}\left(\epsilon_{\gamma}\hat{\rho_{1}}\right) + Re_{\gamma}Pr_{\gamma}\hat{\nabla}\cdot\left(\hat{\rho_{1}}\hat{V_{\gamma}}\right) - \frac{1}{Fo_{\gamma}}\frac{t_{c}}{\rho_{\infty}}\langle\dot{m}\rangle = \frac{Pr_{\gamma}}{Sc}\hat{\nabla}\cdot\left[\hat{\rho_{\gamma}}\hat{\nabla}\left(\frac{\hat{\rho_{1}}}{\rho_{\gamma}}\right)\right]$$
(3.42)

$$\frac{1}{Fo_{\gamma}}\frac{\partial}{\partial\hat{t}}\left(\epsilon_{\gamma}\hat{\rho}_{1}\right) - \frac{1}{Fo_{\gamma}}\frac{t_{c}}{\rho_{\infty}}\langle\dot{m}\rangle = 0$$
(3.43)

$$\frac{1}{Fo_{\gamma}}\frac{\partial}{\partial\hat{t}}\left(\epsilon_{\gamma}\hat{\rho_{1}}\right) + Re_{\gamma}Pr_{\gamma}\hat{\nabla}\cdot\left(\hat{\rho_{1}}\hat{\vec{V_{\gamma}}}\right) = \frac{Pr_{\gamma}}{Sc}\hat{\nabla}\cdot\left[\hat{\rho_{\gamma}}\hat{\nabla}\left(\frac{\hat{\rho_{1}}}{\rho_{\gamma}}\right)\right]$$
(3.44)

3.2.4 Reynolds number estimate

To classify the porous media flow properly it is necessary to estimate the Reynolds number. The properties used to calculate the Re (air density and dynamic viscosity) were evaluated at the air inlet maximum temperature (51.8 °C) to calculate a maximum possible value of this dimensionless number. The mean pore diameter was used as the flow characteristic length for this estimate, which is shown in Eq. (3.45).

$$Re = \frac{\left(1.09\frac{kg}{m^3}\right)(.0018\,m/s)(1.75x10^{-6}\,m)}{.0000196\,kg/m-s} = 2.86x10^{-4}$$
(3.45)

As we can see from the result presented in Eq. (3.45) the porous media flow is characterized by a small Reynolds number (Re << 1). This gives grounds to our assumptions of a quasi-steady flow within the Darcy regime.

3.2.5 Funicular Stage Time Scale

As mentioned previously throughout this study, the drying process of a porous media consists of different stages, each one influenced by different phenomena. In our study, we have mentioned two characteristic stages mentioned in the literature; the initial (funicular) stage driven by the vaporization process and the latter (pendular) stage which is driven by the convective-diffusive transport of energy

and mass. In this section, the calculation of the characteristic time of the initial stage is presented. To do so we will make reference to the work of Whitaker [22], in which it is stated the the characteristic time associated with transport in porous media is on the order of d^2/v_{γ} . In this expression, *d* is the characteristic flow diameter and v_{γ} is the kinematic viscosity of the air. For the early stage, we will determine both a convection and a diffusion time scale, since together these two summarize the time scale for transport at any location. For the time scale of the diffusive transport phenomena we will use the mean grain diameter (D_g) as our characteristic length scale. Likewise, for the convective transport phenomena we will use the mean pore diameter (D_e). The reason for these selections is that diffusion is assumed to occur mainly at the solid region (including the micro-pores) while convection will take place in the void space between grains. The early stage convective time scale will be denoted as t_1 , while the early stage diffusive time scale will be denoted as t_2 . Their formulation and estimate is shown in Eqs. (3.46) and (3.47). For these calculations the properties (density and dynamic viscosity) will be averaged in the entire computational domain.

$$t_1 = \frac{\langle \bar{\rho} \rangle^{\gamma} \cdot D_e^2}{\langle \mu_{\gamma} \rangle} = \frac{(583.8 \ kg/m^3)(0.0147 \ m)^2}{1.8447 \text{x} 10^{-5} \ kg/m - s} = 6838.7 \ s \tag{3.46}$$

$$t_2 = \frac{\langle \bar{\rho} \rangle^{\gamma} \cdot D_g^2}{\langle \mu_{\gamma} \rangle} = \frac{(583.8 \ kg/m^3) (7.87 \text{x} 10^{-3} m)^2}{1.8447 \text{x} 10^{-5} kg/m - s} = 1960.1 s$$
(3.47)

3.2.6 Pendular Stage Time Scale

For the estimate of the latter (pendular) stage time scale we will follow the same procedure used for the time scale of the early stage (Section 3.2.5). The latter stage convective time scale will be denoted as t_3 , while the latter stage diffusive time scale will be denoted as t_4 . Their formulation is presented in Eqs. (3.48) and (3.49).

$$t_{3} = \frac{\langle \bar{\rho} \rangle^{\gamma} \cdot D_{e}^{2}}{\langle \mu_{\gamma} \rangle} = \frac{(584.4941 \ kg/m^{3})(0.0147 \ m)^{2}}{1.8447 \text{x} 10^{-5} \ kg/m - s} = 6846.8 \ s \tag{3.48}$$

$$t_4 = \frac{\langle \bar{\rho} \rangle^{\gamma} \cdot D_g^2}{\langle \mu_{\gamma} \rangle} = \frac{\left(584.4941 \ kg/m^3\right) \left(7.87 \times 10^{-3} m\right)^2}{1.8447 \times 10^{-5} kg/m - s} = 1962.5 s$$
(3.49)

As stated in our assumptions (section 2.4), the characteristic time of our drying process is big enough to assume it is a quasi-steady process. This is in agreement with Whitaker [22], in his statement that the characteristic time of dehydration phenomena is usually in the order of minutes or hours. It is noticeable that the intrinsic phase average density of the gas phase is very high. This happens because of the compressibility of the gas phase and also because the intrinsic phase average uses the volume of the phase instead of the total volume. Based on these calculations we concluded that a time step in the order of minutes is reasonable for our dehydration process.

3.3 Solution Strategy – Flowchart

To solve the coupled system of equations that describes our model it is important to specify the general solution strategy that will be employed. The first detail that will be pointed out is that the equations will be solved in a segregated way. This means that, although coupled, the equations will be solved independently. With the solution of each equation the transport quantities will be updated and used to solve the next equation. This process will be repeated iteratively until all the equations are simultaneously satisfied. Only then, we will be able to move forward in time to keep modeling our drying process. Before presenting the selected numerical methods it is important to have a clear understanding of the sequence in which the equations will be evaluated and what will be the variable updated using that equation as shown in Figure 3.3.1 and Figure 3.3.2.

Obtain
$$\langle T \rangle$$
 \blacktriangleright $\langle \rho \rangle c_p \frac{\partial \langle T \rangle}{\partial t} + \left[\rho_\beta (c_p)_\beta \vec{V}_\beta + \langle \rho_\gamma \rangle^\gamma \langle c_p \rangle^\gamma \langle \vec{V}_\gamma \rangle \right] \cdot \nabla \cdot \langle T \rangle = \nabla \cdot \left[K_{eff} \nabla \langle T \rangle \right] - \langle \dot{m} \rangle \Delta h_{vap}$

Obtain
$$\langle \vec{V}_{\beta} \rangle$$
 \blacktriangleright $\langle \vec{V}_{\beta} \rangle = -\left(\frac{\epsilon_{\beta}\xi\lambda_{\beta}}{\mu_{\beta}}\right) \cdot \left[k_{\epsilon}\vec{\nabla}\epsilon_{\beta} + k_{\langle T \rangle}\vec{\nabla}\langle T \rangle - (\rho_{\beta} - \rho_{\gamma})\vec{g}\right]$

Obtain
$$\langle \vec{V}_{\gamma} \rangle \longrightarrow \langle \vec{V}_{\gamma} \rangle = -\left(\frac{\lambda_{\gamma}}{\mu_{\gamma}}\right) \left[\vec{\nabla} \langle P_{\gamma} - P_{0} \rangle^{\gamma} - \rho_{\gamma} \vec{g}\right]$$

Obtain
$$\epsilon_{\beta}$$
 \longrightarrow $\frac{\partial \epsilon_{\beta}}{\partial t} + \nabla \cdot \langle \vec{V}_{\beta} \rangle + \frac{\langle \dot{m} \rangle}{\rho_{\beta}} = 0$



Obtain $\langle \rho_{y} \rangle^{y}$ \longrightarrow $\frac{\partial [\langle \epsilon_{y} \langle \rho_{y} \rangle^{y}]}{\partial t} + \nabla \cdot [\langle \rho_{y} \rangle^{y} \langle \vec{V}_{y} \rangle] = \langle \vec{m} \rangle$ Obtain $\langle \rho_{1} \rangle^{y}$ \swarrow $\langle p_{1} \rangle^{y} = \langle \rho_{1} \rangle^{y} R_{1} \langle T \rangle$ Obtain $\langle \rho_{2} \rangle^{y}$ \blacktriangleright $\langle \rho_{y} \rangle^{y} = \langle \rho_{1} \rangle^{y} + \langle \rho_{2} \rangle^{y}$ Obtain $\langle p_{2} \rangle^{y}$ \land $\langle p_{2} \rangle^{y} = \langle \rho_{2} \rangle^{y} R_{2} \langle T \rangle$ Obtain $\langle p_{y} \rangle^{y}$ \land $\langle p_{y} \rangle^{y} = \langle p_{1} \rangle^{y} + \langle p_{2} \rangle^{y}$ Obtain $\langle m \rangle$ \flat $\frac{\partial [\langle \epsilon_{y} \langle \rho_{1} \rangle^{y}]}{\partial t} + \nabla \cdot [\langle \rho_{1} \rangle^{y} \langle \vec{V}_{y} \rangle] - \langle \dot{m} \rangle = \frac{\nabla \cdot [\langle \rho_{y} \rangle^{y} D_{eff} \nabla [\langle \frac{\langle \rho_{1} \rangle^{y}}{\langle \rho_{y} \rangle^{y}}]]$

Figure 3.3.2: Solution Strategy (Part II)

3.4 Finite volume method

The solutions provided by the mathematical model proposed in this work will be numerically studied using the finite volume method. This method is a discretization method based on the integral form of the conservation law. One of the advantages of this method is that it increases the accuracy of the central differences by locating the discretization node at the center of the control volume. Also, it provides a better physical understanding than other methods (such as finite difference method). This mainly because the algebraic quantities that appear throughout the discretization process are approximations of the transport quantities flux at surfaces of the control volume. For a detailed explanation of the method refer to the work of Patankar [45], Versteeg and Malalasekera [43] or Ferziger and Períc [46].

In the solution of the transport equations in porous media we will be dealing with two types of equations. The first type is the linear expressions which can be solved using simple algebraic manipulations. An example of this kind of equation are the thermodynamic relations, such as Eqs. (2.57) to (2.60). The second type is the unsteady equations, which could be either linear or non-linear expressions. Most of our equations, such as the total energy equation (Eq. 2.20), could be classified as non-linear unsteady equations. These expressions require a lot more work than linear relations, and analytical solutions are not expected. An example of the unsteady transport of a quantity φ is presented in Eq. (3.50).

$$\frac{\partial(\rho \varphi)}{\partial t} + \nabla \cdot (\rho \vec{V} \varphi) = \nabla \cdot (\Gamma \nabla \varphi) + S_{\varphi}$$
(3.50)

In the equation above there are four terms that we need to understand and treat numerically. The first term in the left side of Eq. (3.50) is the rate of change of intensive quantity φ . It is followed by the convective term. This term usually represents the non-linear part of an individual expression, since it is the gradient of the product of two undetermined transport quantities (velocity and φ in this example). On the right side of Eq. (3.50) we first have the diffusion term, followed by the source term S_{φ} . Now that we have identified each term we need to decide a proper discretization scheme for the differentials present in each one of them, excluding the source term which is not a differentiated quantity.

3.4.1 Central differencing scheme

The first term we will deal with is the diffusion term. This term represents represents the diffusion driven by the gradient of transport quantity φ . Integrating this term using the finite volume method and applying the divergence theorem will lead us to Eq. (3.51).

$$\int \frac{\partial}{\partial x} \left(\Gamma \frac{\partial \varphi}{\partial x}\right) dV = \left(\Gamma \frac{\partial \varphi}{\partial x} A\right)_{i+\frac{1}{2}} - \left(\Gamma \frac{\partial \varphi}{\partial x} A\right)_{i-\frac{1}{2}}$$
(3.51)

The resultant expression states that net diffusive flux along x-axis incoming to our differential volume is equal to the sum of the diffusive fluxes at the two surfaces of our differential volume along that axis. We can see that the diffusive term depends only on the gradient of transport quantity φ . For a linear term like this we can employ the central differencing scheme without significant error. The only criterion necessary to select a discretization scheme for this term is the conservation of the extensive quantity being transported. Versteeg and Malalasekera [43], call this scheme conservative since it uses consistent expressions and the derivatives are evaluated at the surfaces of the differential volume. An example of the employment of the central differencing scheme for the diffusive terms is shown in Eq. (3.52).

$$\frac{\partial \varphi}{\partial x_{i-\frac{1}{2}}} = \frac{\varphi_i - \varphi_{i-1}}{\Delta x}, \qquad \frac{\partial \varphi}{\partial x_{i+\frac{1}{2}}} = \frac{\varphi_{i+1} - \varphi_i}{\Delta x}$$
(3.52)

Lets now consider the transport equation involving both convective and diffusive terms. If we integrate these terms using the finite volume method we will end up with an expression of the form of Eq. (3.53).

$$\left(\rho V_{x} A \varphi\right)_{i+\frac{1}{2}} - \left(\rho V_{x} A \varphi\right)_{i-\frac{1}{2}} = \left(\Gamma \frac{\partial \varphi}{\partial x} A\right)_{i+\frac{1}{2}} - \left(\Gamma \frac{\partial \varphi}{\partial x} A\right)_{i-\frac{1}{2}}$$
(3.53)

To simplify this equation, lets introduce the convective mass flux per unit area F and the diffusion conductance at cell face D. Both are common parameters used in computational fluid dynamics (CFD). With the substitution of these parameters, presented in Eq. (3.54), and assuming the surface area of all

the CV faces as equal, we can write Eq. (3.53) as Eq. (3.55). However, the assumption of constant surface area will be removed later due to the variations of area in our cylindrical coordinates mesh.

$$F = \rho V_x$$
 and $D = \frac{\Gamma}{\delta x}$ (3.54)

$$F_{i+\frac{1}{2}}\phi_{i+\frac{1}{2}} - F_{i-\frac{1}{2}}\phi_{i-\frac{1}{2}} = D_{i+\frac{1}{2}}(\phi_{i+1} - \phi_i) - D_{i-\frac{1}{2}}(\phi_i - \phi_{i-1})$$
(3.55)

The challenge from the equation above is to find a suitable discretization scheme consistent for both the linear and non-linear terms. Employing a method such as central differencing for the convective terms could result in a solution very far from the expected. The principal reason is that the central differencing scheme gives the same weight to all the fluxes at all the control volume faces. That is not true if the quantity under study depends on the velocity of the transporting fluid. Depending on the direction and magnitude of the fluid flow, the influence of one neighbor node on our control volume could be very different than the influence from the other nodes. Take as an example three aligned nodes (A,B,C) located over a heating element. If the flow is in the direction (C,B,A) is more likely that the properties from C will have a stronger effect on B than the properties of A. The ability of a scheme to account for the effects of direction and magnitude of the fluid flow is called transportiveness. Since the convective terms present in our transport equations depend on the velocity of the fluids in motion, a transportive discretization scheme will be employed in their treatment.

3.4.2 Space discretization scheme selection

A discretization scheme that is conservative, unconditionally bounded and satisfies the transportiveness criterion is the hybrid scheme. This scheme was presented by Spalding [88] and consists on switching the discretization employed depending which phenomenon prevails in our process, either convection or diffusion. To determine the appropriate discretization in each direction the cell Peclet number is introduced. This dimensionless number represents the ratio between the convective flux and the diffusive flux at a single face of our control volume. The cell Peclet number could be evaluated from the expression in Eq. (3.56).

$$Pe = \frac{F}{D} = \frac{\rho V_x}{(\Gamma/\delta x)}$$
(3.56)

The hybrid scheme assumes that for small Peclet numbers (Pe < 2) the transport phenomena could be approximated as pure diffusion. Therefore, for this cases we can employ the central differencing scheme to treat both convective and diffusive terms. On the other hand for large Peclet number (Pe \geq 2), the problem is assumed to be pure convection and the diffusion term in this direction could be set to zero. In this case the convective term is treated using the so-called upwind scheme in which the transport quantity φ at the surface of the CV is set to be equal to the value of this quantity in the node having stronger influence. In the example mentioned before (Section 3.4.1) the value of the transport quantity at the surface between C and B would be set to be equal to the transport quantity at C and the value at the surface between B and A to be equal to B. For a more detailed explanation of the upwind differentiation scheme refer to Versteeg and Malalasekera [43].

3.4.3 Time discretization scheme selection

In the previous sections the discretization schemes that will be used to deal with the spatial derivatives is shown. It is now our priority to select a proper methodology to deal with the time derivatives. As we solve this unsteady system of transport equations we will be integrating, and moving, both in space and time. If we integrate Eq. (3.50) over a differential volume and a time step we will obtain an expression in the form of Eq. (3.57).

$$\left[\left[\left[\left[\rho \varphi \right]_{i}^{k+1} - \left[\rho \varphi \right]_{i}^{k} \right] \Delta V + \int_{t}^{t+\Delta t} \left[F_{i+\frac{1}{2}} \varphi_{i+\frac{1}{2}} - F_{i-\frac{1}{2}} \varphi_{i-\frac{1}{2}} \right] dt =$$

$$\int_{t}^{t+\Delta t} \left[D_{i+\frac{1}{2}} \left[\varphi_{i+1} - \varphi_{i} \right] - D_{i-\frac{1}{2}} \left[\varphi_{i} - \varphi_{i-1} \right] \right] dt + \int_{t}^{t+\Delta t} \langle S \rangle_{V} \Delta V dt$$

$$(3.57)$$

As seen from Eq. (3.57) the local change in time has been easily evaluated by expressing the definite integral in terms of the value of the transport quantities at time steps k and k+1. Now, if we do the same with the terms involving spatial derivatives we will introduce the values of the neighbor control

volumes properties at different time steps. Then it will become an unsolvable system, since we can only determine one unknown at the time.

There are three different approaches with which we can deal with this problem. First we could employ an explicit method, in which we assume the transport quantities from the spatial derivatives to be evaluated at old time step k. This would be convenient considering that as we move in time we will always know the old values of the transport quantities (starting from our initial conditions). The second approach is to use an implicit method in which we assume that the transport quantities are evaluated at a future time step within k and k+1. This introduces some numerical complexity, since we don't know the value of the transport quantities for a future time step and the solution of the equations will be only possible via iterative methods. Nonetheless, implicit methods are numerically unconditionally stable. Again the word "numerically" is used to emphasize that this only ensures finding a solution for a wellposed system of equations and does not release us from other numerical instabilities due to the nonlinearity of the process. Using a fully implicit scheme, which means evaluating the spatial derivatives at k+1, could provide further advantages such as ensuring that all our coefficients (at *i*, *i*-1, etc.) have the same sign. This would improve the convergence properties of our system of equations. If we implement the fully implicit scheme to Eq. (3.57) and assume that the average source term is a linear function of the concerning transport quantity it could be written as shown in Eq. (3.58). About the treatment of the source term we will get back in the discussion presented in the next sections.

$$\begin{bmatrix} \left[\left(\rho \,\varphi\right)_{i}^{k+1} - \left(\rho \,\varphi\right)_{i}^{k}\right] \Delta V + \left[\left(F_{i+\frac{1}{2}} \,\varphi_{i+\frac{1}{2}}\right)^{k+1} - \left(F_{i-\frac{1}{2}} \,\varphi_{i-\frac{1}{2}}\right)^{k+1}\right] \Delta t = \\ \begin{bmatrix} D_{i+\frac{1}{2}}^{k+1} \left[\left(\varphi_{i+1} - \varphi_{i}\right)^{k+1} - D_{i-\frac{1}{2}}^{k+1} \left(\varphi_{i} - \varphi_{i-1}\right)^{k+1}\right] dt + \langle S \rangle_{V} \,\Delta V \,\Delta t \end{bmatrix}$$
(3.58)

3.5 Implementation of Space-Time Schemes

For the solution of parchment coffee (*C.Arabica*) dehydration equations, discretization will be done using the hybrid scheme to integrate in space and a fully implicit scheme for time. The former statement means that the temperatures, humidities and other transport quantities will be solved using new variables at time $t+\Delta t$. Consequently, we need to solve the equations iteratively at each time step. This could be computationally expensive, but at the same time our scheme will not require a very small time step to ensure numerical stability. A diagram for the one dimensional solution of a single PDE in our system of equations is shown in Fig. 3.5.1. In the top part of the image we can see how the input values are mainly estimates of the transport quantities at time $t+\Delta t$. As the iteration process moves forward this estimates are refined until all the volume averaged transport equations are simultaneously satisfied. In this diagram (Fig. 3.5.1) we can also see the implementation of the hybrid scheme for the spatial discretization of our transport equations. The first step for this implementation is the accumulation of coefficients from Eq. (3.58) into the algebraic expression in Eq. (3.59). In this equation, is given by Eq. (3.60). To apply the Peclet number criterion we will use the expressions proposed by Versteeg and Malalasekera [43], as shown in Eq. (3.61). Using these expressions it is possible to formulate the value of the neighbor coefficients accounting for the effects of the direction and magnitude of the flow.

$$a_i^{k+1} \varphi_i^{k+1} = a_{i+1}^{k+1} \varphi_{i+1}^{k+1} + a_{i-1}^{k+1} \varphi_{i-1}^{k+1} + a_i^k \varphi_i^k + S^{k+1}$$
(3.59)

$$a_{i}^{k+1} = a_{i+1}^{k+1} + a_{i-1}^{k+1} + \left(F_{i+1}^{k+1} - F_{i-1}^{k+1}\right)$$
(3.60)

$$a_{i+1}^{k+1} = max \left[-F_{i+1}^{k+1}, \left(D_{i+1}^{k+1} - \frac{F_{i+1}^{k+1}}{2} \right), 0 \right], \quad a_{i-1}^{k+1} = max \left[F_{i-1}^{k+1}, \left(D_{i-1}^{k+1} + \frac{F_{i-1}^{k+1}}{2} \right), 0 \right]$$
(3.61)



Figure 3.5.1: Implementation of Discretization Schemes

3.6 Implementation of Boundary Conditions

The formulation of the boundary conditions for our mathematical model has been presented in section 3.1.3. It is now our intention to discuss the numerical implementation of these conditions. It will be done in a vector notation form. However, for the actual implementation in the code developed the reader can refer to Appendix II. The boundary conditions for the temperature field are presented in Eqs. (3.62) to (3.64). In these expressions *i* refers to the radial coordinate of the center of a control volume and *j* refers to the vertical coordinate, both within the domain of a *n* x *m* mesh grid. To evaluate the zero flux boundary conditions Eqs. (3.4) and (3.5) we will generate ghost cells at position *i*=1, *i*=n and *j*=m. This cells will be outside of our physical domain (at a distance $0.5\Delta r$ or $0.5\Delta z$ from our boundaries) and their properties will be set to be equal to their neighbors to force a zero flux condition at these surfaces. This is clearly shown in Eqs. (3.63) and (3.64). It must be pointed out that these conditions are truth for $k \neq 0$.

$$T_{i,j=1}^{k} = T_{SA} (3.62)$$

$$T_{i=1,j}^{k} = T_{i=2,j}^{k}, \quad T_{i=n,j}^{k} = T_{i=n-1,j}^{k}$$
(3.63)

$$\Gamma_{i,j=m}^{k} = T_{i,j=m-1}^{k}$$
(3.64)

At t = 0 the coffee bed is at a temperature $T_0 = 23$ °C. The implementation of this condition is shown in Eq. (3.65).

$$T_{i,j}^{k=0} = T_0 \tag{3.65}$$

Using the same notation, the boundary conditions for the liquid motion are presented in Eqs. (3.66)-(3.68). The conditions in Eq. (3.66) represent the no-slip conditions applied to the cells at the boundaries of the domain. As explained earlier, the Neumann boundary conditions (flux boundary conditions) are imposed by generating a series of ghost cells. This is shown ins Eq. (3.68) were we use a ghost cell (i, m) to set the change in velocity at the boundary to zero.

$$\langle u_{\beta} \rangle_{i=2,j}^{k} = 0, \quad \langle u_{\beta} \rangle_{i=n-1,j}^{k} = 0, \quad \langle w_{\beta} \rangle_{i=2,j}^{k} = 0, \quad \langle w_{\beta} \rangle_{i=n-1,j}^{k} = 0$$

$$(3.66)$$

$$\langle u_{\beta} \rangle_{i, j=1}^{k} = 0, \quad \langle w_{\beta} \rangle_{i, j=1}^{k} = 0$$
 (3.67)

$$\langle u_{\beta} \rangle_{i, j=m}^{k} = \langle u_{\beta} \rangle_{i, j=m-1}^{k}, \quad \langle w_{\beta} \rangle_{i, j=m}^{k} = \langle w_{\beta} \rangle_{i, j=m-1}^{k}$$
 (3.68)

The initial condition for the liquid phase velocity field is shown in Eq. (3.68).

$$\langle u_{\beta} \rangle_{i,j}^{k=0} = 0, \quad \langle w_{\beta} \rangle_{i,j}^{k=0} = 0 \tag{3.69}$$

With the same reasoning as that used for the implementation of β -phase boundary conditions, the boundary conditions and the initial condition for the gas motion are presented in Eqs. (3.70) to (3.73).

$$\langle u_{\gamma} \rangle_{i=2,j}^{k} = 0, \quad \langle u_{\gamma} \rangle_{i=n-1,j}^{k} = 0, \quad \langle w_{\gamma} \rangle_{i=2,j}^{k} = 0, \quad \langle w_{\gamma} \rangle_{i=n-1,j}^{k} = 0$$

$$(3.70)$$

$$\langle u_{\beta} \rangle_{i, j=1}^{k} = 0, \quad \langle w_{\beta} \rangle_{i, j=1}^{k} = \frac{C_{entrance} \cdot Q_{fan}}{A_{SA}}$$

$$(3.71)$$

$$\langle u_{\gamma} \rangle_{i,j=m}^{k} = \langle u_{\gamma} \rangle_{i,j=m-1}^{k}, \quad \langle w_{\gamma} \rangle_{i,j=m}^{k} = \langle w_{\gamma} \rangle_{i,j=m-1}^{k}$$
 (3.72)

$$\langle u_{\gamma} \rangle_{i,j}^{k=0} = 0, \quad \langle w_{\gamma} \rangle_{i,j}^{k=0} = 0 \tag{3.73}$$

Finally, the numerical implementation of the initial conditions for the volume fractions is shown in Eq. (3.74)-(3.75). At the air inlet (*j*=1) the volume fraction of liquid is zero. Although Eq. (3.13) shows that the initial condition of the liquid volume fraction is a function of the moisture content, if we assume the porous media to be completely saturated at *t*=0, the liquid volume fraction would be equal to the porosity.

$$\langle \epsilon_{\beta} \rangle_{i,j=1}^{k} = 0 \quad \langle \epsilon_{\beta} \rangle_{i,j=1}^{k=0} = \varphi$$
(3.74)

$$\langle \epsilon_{\gamma} \rangle_{i,j=1}^{k} = 1 \quad \langle \epsilon_{\gamma} \rangle_{i,j>1}^{k=0} = 0$$

$$(3.75)$$

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3.7 Mass Conservation Verification at Pressure Outlet

The verification of the conservation of mass at the pressure outlet as discussed in section 3.1.3 is implemented in Eq. (3.76). In this expression we calculate the residual volumetric flow. Physically, the gas phase volumetric flow at the pressure outlet must be equal to the inlet volumetric flow plus the total vaporization per unit volume. In Eq. (3.77) we uniformly distribute the residual flow calculated at Eq. (3.76) to comply with the conservation of mass principle. This is done by correcting the γ -phase velocity at the outlet.

$$\dot{V}_{residual} = \sum_{i=1}^{N} \left[\langle w_{y} \rangle_{i,j=1}^{k} A_{j} \right] + \sum_{i=2}^{n-1} \sum_{j=2}^{m-1} \langle \dot{m} \rangle_{i,j}^{k} - \sum_{i=1}^{N} \left[\langle w_{y} \rangle_{i,j=m}^{k} A_{j} \right]$$
(3.76)

$$\langle w_{\gamma} \rangle_{i,j=m}^{k} = \langle w_{\gamma} \rangle_{i,j=m}^{k} + \frac{\dot{V}_{residual}}{(n-2)A_{j}}$$
(3.77)

3.8 Numerical Solution – Flowchart

Throughout this chapter we have discussed the development and implementation of a numerical method to solve our coupled system of equations. This method was applied in a MATLAB code written with the solely purpose of demonstrating the capabilities of our mathematical model and comparing our solutions with experimental results obtained for this study. In the flowchart presented on Fig. 3.8.1 the different subroutines operating inside this code and their functions are illustrated. The parameters concerning the mesh generation, time duration of the simulation and thermophysical correlated properties are read by the code from input files. This information is used to generate the mesh and create an initial vector of transport quantities based on the initial conditions. When relating the transport quantities to a vector we must recall that at the end we will end up solving a matrix system (Ax = y) for each PDE. In this system the transport quantities at any location are contained in the column vector x. These vectors are then used as an estimate of the future transport quantities (at $t+\Delta t$). The next step is to generate the coefficients matrix A and the solution column vector y for our transport equations based on the selected discretization schemes. These arrays are sent to the solver, which uses the bi-conjugate gradient stabilized method to provide a solution.

homogeneous 2-D system of equations the resultant array of coefficients is a pentadiagonal sparse matrix. This solution vector is used to update the estimate of the future transport quantities. After all the equations are solved the algorithm verifies if there was any change in the variables with respect to the previous estimate. If the total residual in changes was greater than 1.0 E-4 for any variable, the iterative process continues. Once all the equations are satisfied simultaneously (total residuals less than 1.0 E-4) the solutions are written into a time labeled output file and the time step moves forward to continue our simulation.



Figure 3.8.1: MATLAB Code Flowchart

4 **Results and Discussion**

Using the mathematical model discussed in Chapter 2 and the numerical solution method proposed in Chapter 3 we were able to predict the dynamics of temperature and moisture content throughout the dehydration process of parchment coffee. This was done at a certain degree of accuracy which is a direct result of the assumptions done in our modeling as well as the controllability of the experimental data acquisition. This chapter is devoted to the presentation and discussion of the results obtained.

4.1 Experimental Results using HARC²S

A series of experiments was performed using the HARC²S as discussed in the materials and methods presented on Chapter 1. This system, designed and built by Dr. Francisco Rodríguez Robles and Dr. Francisco Monroig Saltar [8], was used to obtain temperature and moisture content data during five different dehydration processes. Four of these experiments were done using the capability of air recirculation provided by the HARC²S and one experiment was performed discharging the air without any recirculation. The four experiments using air recirculation are referred in this study as closed batea (CB) and the experiment done without recirculation as open batea (OB). A temperature sensor as that shown in Fig. 1.5.2 was located inside the parchment coffee bed at a height of 0.18 m (7 in) and a radius of 0.152 m (6 in). The following images are two examples of the data obtained for the coffee mass temperature and moisture content using either closed batea or open batea configuration.



Figure 4.1.1: Experiment configurations Open Batea (OB) and Closed Batea (CB)



Figure 4.1.2: Experimental Data of Dehydration Dynamics (CB1)



Figure 4.1.3: Experimental Data of Dehydration Dynamics (OB2)

Due to the nature of the experiment, and the selected data acquisition method, the obtained temperature data is limited to the behavior of the coffee mass temperature at a single position. For the moisture content the coffee mass sample were randomly taken from the exposed coffee bed surface. This selection increases the probability of our sample of being a better representation of the average conditions. Now, understanding these limitations it is clear that the accuracy of our temperature prediction can only be determined in terms of proximity to the experimental value at the specific location of the temperature sensor. Likewise, the moisture content prediction can only be compared at an average level.

Analyzing the relationship between the coffee mass temperature and the supply air temperature could provide important information about the phenomena itself. In Fig 4.1.3 we can appreciate how the coffee mass temperature and air supply temperature behave for a specific configuration.



Figure 4.1.4: Heat Transfer Coffee Mass Resistance (CB1)

As we can see from Figure 4.1.3, at the beginning of the dehydration process, the coffee mass temperature increases even higher than the supply temperature. This is expected since the coffee bed is saturated with water. Given that the water has a higher heat capacity than the air, it delays the heat release from the coffee mass causing an increment in temperature. We could say that the presence of water causes the porous body to accumulate energy as shown by the coffee mass temperature rise. As we move to the completion of the first hour of our drying process, the temperature of the coffee mass becomes smaller than the temperature of the supply air. This is not because of the reduction of the moisture content since it has only started decreasing. The reason for this phenomenon is the so-called evaporative cooling. Due to the vaporization of water at the surface of the coffee grains, the coffee mass is loosing some of the heat delivered by the gas phase. Once the supply air has basically reached the setup temperature (at approximately 1.2 hours) an unexpected coffee mass temperature reduction occurs. The initial hypothesis for this occurrence was that it was a combination of the evaporative cooling and the arrival of a steady supply air temperature condition. However, as shown in Fig. 4.1.4, this occurrence is not repeated in any of the other experiments. This lead us to conclude that it represents some sort of environmental disturbance such as raining incidence. Stating that this is not a phenomenological characteristic of our process is important to evaluate the quality of the model developed in this study. Another important comment on the comparison between coffee mass temperature and supply air temperature is that at the end of the process they coincide. This is primarily due to the fact that we arrived to a steady state condition and the water resistance in our porous body is not significant anymore. In the next section we present a comparison between the mathematical model and the empirical data.



Figure 4.1.5: Experimental Results Comparison

4.2 Numerical Results

The main objective of this study is to develop a mathematical model able to predict the dynamics of temperature and moisture content throughout the concerning drying process. To evaluate the accuracy of our model, the simulated data was plotted against the experimental data. Doing this comparison for different assumptions and cases enhances the understanding of the driving forces behind each of the stages of our process. The first simulation presented below (Fig. 4.2.1) is the drying process using an open batea configuration.



Figure 4.2.1: Resulting Dynamics of Dehydration (OB2)

It is important to recall that for convergence purposes and to decrease the computational cost the modeling will be divided into two stages as proposed in section 2.3.3. The first stage will not consider convective fluxes due to the saturation level of the coffee mass as shown in Eq. (2.29) and the second stage will not consider the vaporization sink terms as done in Eq. (2.30). To switch between these two models the understanding provided by the empirical data was used. If we observe the drying curves of all our experimental cases we can observe that the temperature nonlinear behavior is limited to the first 2 hours of dehydration and the final hour of dehydration.

The first non-linear section could be attributed to the vaporization of water. The volume occupied by water is reducing dramatically, introducing phase discontinuities (or jumps) into the macro-pore volume. Due to the difference between the heat capacity of air and water the

temperature increases in a nonlinear way until the macro-pore section is basically dry and the water left is inside the coffee beans (micro-pores). At this point, the macro-pores are filled with moist-air and the flow becomes continuous in terms of intrinsic phase average density of air. From that point on, the γ -phase flow becomes organized and the convective heat transfer becomes significant in the behavior of the coffee mass temperature. In Figures 4.2.2 – 4.2.9 we can see the coffee mass temperature distribution as it develops throughout the entire drying process of the selected configuration (OB2). While these images are contour plots and have little use for validation purposes, it will give us some important insights of the phenomena under study and how well our model capture certain characteristics of the process.



Figure 4.2.2: Temperature Distribution at t=0.27 hrs (OB2)



Figure 4.2.3: Temperature Distribution at t=1.0 hrs (OB2)



Figure 4.2.4: Temperature Distribution at t=1.5 hrs (OB2)



Figure 4.2.5: Temperature Distribution at t=2 hrs (OB2)



Figure 4.2.6: Temperature Distribution at t=4 hrs (OB2)



Figure 4.2.7: Temperature Distribution at t=6 hrs (OB2)



Figure 4.2.8: Temperature Distribution at t=8 hrs (OB2)


Figure 4.2.9: Temperature Distribution at t=9 hrs (OB2)

In Figure 4.2.2 it is shown how at the beginning of the drying process the air inlet (bottom of the contour plot) has a very small effect in the temperature changes of the body. This image is taken around 15 minutes after the drying started and the temperature of the coffee mass is still very close to the initial temperature (23 °C). Also, we can see how the contours are almost straight due to the little influence. If the flow passing through the macro-pore were significant we would be able to see the radial effects on the temperature distribution. The studied volume is a cylinder, therefore as we approach the center (r=0) the control volume becomes smaller and the conduction heat transfer is smaller. At this point of the process we still cannot see this effect because of the saturation level. As the saturation level decreases we expect the mass weighted averaged heat capacity to become smaller (since water has a higher specific heat) and the heat transfer rate to increase. This result is replicated in Figure 4.2.1 were the model temperature behavior is first concave downwards and as the saturation level decreases it becomes concave upwards. Some discrepancies exist between our model and the experimental data which gives notion of multiple inflection (more than one change of concavity). After the inflection occurs and

the heat transfer rate increases, the radial effects of heat transfer must be evident. This is clearly shown on Figure 4.2.3 where the temperature contours are shaped like positive parabolic functions.

The heat transfer rate will reduce as we get close to the linear region of the process since the temperature gradient becomes almost negligible. In Figure 4.2.5 we can see some blurry contours, and if we pay attention to the legend we will realize that the maximum temperature gradient is of the order of one hundredth of a degree. This helps to explain why the temperature response becomes almost linear after this point (see Figure 4.2.1). It is clear that the rate of change of temperature will depend strongly on the convection fluxes, while the diffusion and vaporization fluxes influence will be minimal. This will be true until the steady stage is reached. As it can be seen in Figure 4.2.1, the behavior of the model temperature response is very similar to a first order system that reaches its steady value within the first 2 hours of drying. This is different to the real behavior which delays its arrival to equilibrium until the end of the process. One of the possible reasons for this difference is the assumption of a constant pressure gradient which pushes the air velocity to be relatively constant. This comparison between our model's predictions and the experimental data seems to be very consistent for different drying conditions as seen on Figures 4.2.10 to 4.2.13. A comparison between the predictions of the proposed model and the predictions of the model published by Rodriguez-Robles [51] is presented on Figure 4.2.14.



Figure 4.2.10: Resulting Dehydration Dynamics (CB1)



Figure 4.2.11: Resulting Dehydration Dynamics (CB2)



Figure 4.2.12: Resulting Dehydration Dynamics (CB3)



Figure 4.2.13: Resulting Dehydration Dynamics (CB4)



Figure 4.2.14 Dehydration Dynamics Model Comparison

Each one of the five different simulated cases shown above present the same discrepancy with the experimental temperature. However, all of them present fairly good predictions of the moisture content; especially at equilibrium. In the next section we present a short summary of the deviation of our results from the actual data. This will be done at fixed locations as explained at the beginning of this chapter.

4.3 Statistical Analysis

The percent of difference between the experimental data and our predicted values was calculated for all of the cases. This difference is defined as the ratio of the difference between the experimental data and the predicted values to the average between these two. A calculation example for the temperature percentage difference is shown in Eq. (4.1). The mean and standard

deviation of the percentage difference of both temperature and moisture content is presented in Tables 4.3.1 and 4.3.2.

$$\% diff_{T} = \frac{|T - T_{exp}|}{\frac{1}{2} (T + T_{exp})}$$
(4.1)

Case	Temperature Mean % diff	Temperature % diff Stdev
OB2	6.88	5.12
CB1	9.53	8.85
CB2	10.32	7.18
CB4	9.50	9.25
CB4	9.48	8.07

Table 4.3.1: Temperature Percentage Difference Statistics

Case	M.C. (%w.b.) Mean % diff	M.C. (%w.b.) % diff Stdev
OB2	23.73	11.99
CB1	9.40	7.98
CB2	18.60	11.20
CB4	10.30	7.25
CB4	8.83	7.21

Table 4.3.2: Moisture Content Percentage Difference Statistics

As it can be seen by comparing the last two tables, the error of these predicted values could be as high as 30 %. From these statistics, it seems to be that the model is better predicting temperature than moisture content. However, these conclusions should not be taken so fast. The former statement is only true if the error (percentage difference) distribution of our results is

perfectly Gaussian. Since the equations and assumptions behind our model are not the same through the entire simulation, it is to be expected to have a non-Gaussian error distribution. This characteristic is common of step-wise like models as the one proposed in this study. As it will be shown in the images below this is found to be true for our simulation. An example distribution of the percentage difference of moisture content is presented in Figures 4.3.1 and 4.3.2 for two different cases. In the first image (case CB1), the percentage difference of the moisture content remains below 10 % for the first seven hours of dehydration, increasing at the last stage up to a percentage difference of 24.8 %. On the other hand, in the second image (case CB4) the percentage difference stays below 10 % most of the drying process with the exception of the fourth and fifth hours. We can notice from the histograms below that both cases behave far from a normal distribution.



Figure 4.3.1: M.C. Percentage Difference Distribution (CB1)



Figure 4.3.2: M.C. Percentage Difference Distribution (CB4)

The reason for this non-Gaussian behavior is not only the phenomena switching but also the given test conditions. Due to the nature of the measurement, the moisture content sampling resolution is limited. As mentioned earlier in this study, from the law of large numbers we understand that the average of a sample becomes representative of the population average as we increase the number of samples itself. That is not the case of the moisture content which was experimentally measured at a rate of one sample per hour.

Now, for the evaluation of our coffee mass temperature predictions the resolution is not a problem since it was measured every minute throughout the entire experiments. The temperature percentage difference for this two cases is shown in Figures 4.3.3 and 4.3.4. As expected from the results presented in the previous section, the highest percentage differences occur at the initial drying stage and the discrepancies reach a maximum close to the end of the first hour, when the phenomena switching is most likely to happen. Once the drying rate decreased substantially and

the convective-diffusive stage takes place, the percentage differences become smaller. If we observe the histograms below we will see that the temperature percentage difference distribution is also non-Gaussian. This can be attributed to the high error incidences in the initial stage, the phenomena switching and the assumptions imposed to estimate some of the transport coefficients. About the effect of the transport coefficient is important to clarify that not all of them are function of the same variables. If, as an example, our coefficients were only temperature dependent we would expect to have a normal error distribution, function of the error of the predicted temperature (given that each coefficient's correlation is accurate). However, some of our coefficients depend on temperature, others depend on moisture content and others depend on multiple transport quantities.



Figure 4.3.3: Temperature Percentage Difference (CB1)



Figure 4.3.4: Temperature Percentage Difference (CB4)

4.4 Drying Rate Estimate

One of the challenges related to the modeling of any dehydration process is the prediction of the drying rate. A lot of research effort is concentrated in the modeling of the drying rate as a function primarily of temperature and equilibrium moisture content [16, p.1676]. As mentioned at the beginning of chapter 2, and shown in Figure 2.1, the drying rate could be used to identify the transition between the two drying stages. In the initial (funicular) stage the changes in drying rate are small enough to consider it to be constant. Otherwise, at the latter (pendular) stage the drying rate decreases almost linearly. To study the drying results we will consider one of the dehydration cases. In Figure 4.4.1 the behavior of the drying rate throughout these drying process

is presented. The initial behavior of the drying rate is common to some drying processes and is denominated as the initial transient. Due to the reduction of the saturation level, the drying rate shows a high slope reduction during the first half-hour of dehydration. This high slope reduction finishes with an evident inflection point, which could be attributed to the dehydration of the macro-pore region. Since the parchment coffee mass was initially saturated the air is not able to flow through the macropores until the saturation level decreases to a certain amount. Once the air starts flowing through the void space, the energy input at the inlet is not used uniquely for vaporization anymore. Now, part of the energy delivered to the coffee mass will be transferred to the air as part of the fluid-surface interaction. At the same time the temperature gradients start becoming smaller as discussed in section 4.2. This reduction in the temperature gradient affects negatively the migration of water to the surface (due to the Soret effect) leading to a stabilization of the drying rate. In other words, the non-linear terms depending on the temperature gradient become negligible and the drying rate becomes linear as a consequence. This linear behavior is expected and thoroughly studied due to its simplicity advantages [16, p.1677]. As seen in Figure 2.1, we expected the behavior of the drying rate to be linear at the latter stage. Our results regarding the relationship between the drying rate and the moisture content (Figure 4.4.2) are validated by this drying theory.



Figure 4.4.1: Drying Rate Characterization (CB1)



Figure 4.4.2: Relationship Between Drying Rate and M.C. (%d.b.)

5 Conclusions

The complexity of modeling the dehydration process of a porous media can be divided in three wide groups: formulation constraints, transport coefficients estimate and numerical stability. Most of the discrepancies with the empirically obtained data could be assigned to one of these. For a better sequential presentation of our conclusions, they will be separated based on the phenomenological time frame. First, we will present the conclusions on our predictions over the funicular state, followed by the conclusions related to the pendular state.

5.1 Discrepancies on Funicular State

The funicular state is driven by the phase change phenomenon (primarily vaporization) at the liquid-gas interface. Therefore, the accuracy of the predictions depend on the ability of our model to predict the vaporization rate. One of the disadvantages of the proposed model is that the prediction of the vaporization rate is based solely on the local change of energy. This means that the vaporization rate is calculated as the ratio of the local rate of change of energy to the temperature gradient. A more accurate and phenomenologically correct formulation would have to include the change of energy due to mass diffusion. The former phenomenon is known as the Dufour effect and is included in the formulations of heat and mass transfer in capillary porous bodies presented by Luikov [21]. This was excluded from the original formulations due to problems regarding the stability of our numerical solution. This instability issue summarizes one of the greatest limitations of the methodology selected. Since the volume average method considers all quantities in an average sense, it fails in predicting the distribution of moisture. In other words, given that both the concentration gradient and the diffusivity are very small quantities, the mass fluxes become practically zero after the averaging process. The solution to this issue is clear, though. Increasing the mesh resolution will improve the predictions by

decreasing the uncertainty due to volume averaged space. However, decreasing the volume averaged size will result in a numerically unstable solution. The reason for this instability is that our mesh volume size will be too close to the representative element volume (REV). Close to (or under) the REV, our analysis scale would be affected by random pore scale heterogeneity causing our results to fluctuate from iteration to iteration without converging. To substantiate this conclusion, the REV sizes determined by Constanza-Robinson [48] were compared to the volume averaged size used in our model. This was studied for different mesh resolutions. It was determined that for mesh finer than 100x100 nodes the volume averaged sized is smaller than the referenced nominal REV calculation.

5.2 Discrepancies on Pendular State

The pendular state is driven by the convection-diffusion phenomena. The mechanism of water removal is still vaporization, but the time scale of this process is a lot slower than the transfer of energy due to convection at the macro-pore interface. Observing the results as the system gets closer to the steady state conditions, the accuracy of the predictions improve. This implies that the energy transfer in the latter drying stage could be properly modeled as solely convectiondiffusion heat transfer. The small discrepancies present in this stage could be attributed to errors in the modeling of the convective heat transfer and errors in the estimate of topological parameters. While modeling the convective phenomenon it was assumed that the effects of convective fluxes were only significant in the equations of continuity. This constraint was introduce given that the volumetric effects are expected to be much greater than the surface interaction at the macro-scale. In spite of that, neglecting these effects introduces some error in our predictions since the absence of convection heat transfer increases the conduction heat transfer rate. Not having any convection resistance, the coffee mass temperature increases at a faster rate than the observed (measured) temperature. Considering the convective heat fluxes could be an option to improve our predictions. Even though, some modifications must be done to the model to account for flow direction effects. As concluded by Pierre [49] the volume averaged method convergence is guaranteed only for unidirectional velocity fields. However, on the steady state he concluded: "concentrating on the stationary solution associated with large Peclet numbers, it has been found that volume averaging methods converge toward the exact solution". This agrees with the results obtained using our model; the closer to equilibrium, the better the predictions.

5.3 Recommended Usage

The mathematical model proposed in this work is accurate in predicting the equilibrium conditions as well as the average transport quantities. Therefore, it is within these limits that its use is recommended. This model should be used as a tool to determine the equilibrium moisture content and the time required to obtain that state. The predicted temperature could be post-process to determine the energy input necessary to satisfy a predetermined equilibrium criteria using a specific machinery configuration. Additional to energy, other integral quantities could be accurately determined using this model such as volumetric air flow, total mass evaporated and average moisture content. This model should not be used with the intention of capturing microscale dynamics for the reasons discussed in previous sections. As will be proposed in the following section, this model could be employed as a low-level (macro-scale) predictor to provide boundary conditions to a high level (micro-scale) mathematical model.

5.4 Recommended Drying Process Parameters

The understanding of this dehydration process facilitates the selection of drying parameters that will promote coffee mass moisture transport during dehydration with minimal energy input. Based on this study, it is impossible to optimize this drying process with a unique combination of parameters. To effectively promote moisture transport during the entire dehydration process, the drying parameters should adapt adequately to the two different stages inherent to this process. At the beginning of the drying process, the coffee mass is saturated in water and the air flow effective area is minimum. Therefore, it is recommended to set the inlet air velocity (fan speed) to a minimum. In contrast, at this early stage it is recommended to set the temperature to a maximum level to overcome the resistance represented by the high specific heat of water. However, once the coffee mass has reached a temperature close to the air inlet temperature, the temperature of the air should be reduced to prevent burning the coffee beans close to the inlet. The secondary stage of this process (pendular state) is mainly driven by convective heat transfer. At this point in the dehydration process there is no significant resistance from the moisture content in the macro-pore region. This implies that the air is now able to flow inside the macropores developing a velocity profile and that the heat can distribute easier throughout the coffee mass. Thus, it is recommended to set the fan speed to a maximum. At this stage the temperature should be set to an average value because the drying process in the pendular state is dominate by convection heat transfer. Using a high temperature setting will have a small effect on the process, since the coffee mass temperature distribution is uniform and the mean value is close to the steady state temperature of the process. From an energetic point of view, the use of high temperature air flow at the latter stage of a drying process entails significant energy inefficiency.

5.5 Future Work

This study does not pretend to model all the scales involved in the drying of a porous medium. The objective of this work was to predict the dynamics of temperature and moisture content as well as understanding the contribution from the responsible physical phenomena. Due to the limitations and constraints inherent to the methodology selected, this study was performed only at the macro-pore level. The next step towards a better modeling of this process is the refinement of the transport coefficients and topological parameters. Both the topological function ξ and the

permeability of the parchment coffee mass could be determined from experiments. Relating Darcy's law with appropriate volumetric flow rate calculations, the permeability tensor could be determined. For the calculation of ξ , the capillary pressure of the porous medium needs to be correlated experimentally. An easy approach for this would be to use the Leverett function. However this will require information regarding the micro-scale flow interactions. For a macro-level, our proposed estimate of the topological function (section 2.6.7) seems reasonable, both physically and numerically. This refinement of parameters will improve our results especially at the transition between functuar and pendular states, since at that point the liquid-gas interactions at the pore channels is most significant.

To accurately analyze the micro-pore level, a different approach must be used. The recommendation is to formulate a multi-scale model. In this methodology a coarse domain (macro-level) is first solved using the volume averaged equations of heat and mass transfer. Then the estimates from this model are entered as boundary conditions into a fine domain (micro-pore) governed by capillary-diffusive phenomena. Again, such approach requires empirical acquisition of parameters such as curvature radii and surface tension. A final comment on micro-scale modeling is that it cannot be accurately modeled using conventional deterministic methods. Reasons for that are the number of unknowns, the uncertainty level for a volume smaller than the REV, and unexpected interactions with the environment. However, a multi-scale model could be randomized and solved repeatedly ("random search") until an accurate solution is obtained via the use of a genetic algorithm such as the Monte Carlo algorithm. Genetic algorithms are suitable to deal with unknown parameters such as the topological function or its related so-called tortuosity tensor. This approach is suggested for the solution of flow in porous media by S.D. Harris [50]. As implied in these recommendations, the selection of a methodology to model a dehydration process will depend on the scale desired, the concerning quantities, and also the data available to obtain parameters unique of our specific porous medium.

6 References

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Appendix I: Matlab Finite Volume Code

%Transient Solution of the Equations of Simultaneous Heat and Mass %Transfer in the Dehydration Process of Parchment Coffee (C. Arabica)

%Author: Moises Y. Ocasio %Adviser: Dr.Francisco Rodriguez %Comittee members: Dr. Orlando Ruiz % Dr. Francisco Monroig

clear all
close all
clc
close all hidden

% Changing directory to Field Data Directory

cd('/home/myobhel/Desktop/Research/MATLAB Code/');

%% I. READING INPUT DATA

%Static Data

P=importdata('param.txt');

T_SA=importdata('CB1/SUPPLY.txt');

A=importdata('CB1/PSAT.d');

II=importdata('CB1/RH1.d');

O=importdata('CB1/RH2.d');

T_Smax=61;

%% II. CREATING MESH

%1-radial, 2-bed height

L1=.32258; L2=.235;

N1=20; N2=20; N3=(N1)*(N2);

DR=L1/(N1-1); DZ=L2/(N2-1);

DRd=1/(N1-1); DZd=1/(N2-1);

D5=[N1 1 0 -1 -N1]; %specifier for pentadiagonal sparse matrix

%% III. INITIAL CONDITIONS

%1.Input Conditions

T_0=23; %Initial Coffee Mass Temperature (Celsius)

W_Y0=0.0018; %Air Inlet Z-Speed (m/s)

 $M_0=.56;$

%General Parameters

G=9.81; %Gravitational Acceleration

DTIME=120; %Time Step in seconds

TTIME=10000; %Total Time in seconds

%Phenomenological Switching

SWITCH1=11;

SWITCH2=11;

ITER=20; %Number of IMPLICIT iterations

KTOTAL=ceil(TTIME/DTIME);

SOR=1E-10; %Ratio of reduction for CGSTAB Solver

R_IDEAL=8.3144621;

MAIR=.0289645; %Kg/mol

MH20=.01801528; %kg/mol

Rallow=.001; %Convergence criteria (Total RMS)

%2.Transport Quantities

T=ones(N2,N1);

U_B=ones(N2,N1);

U_Y=ones(N2,N1);

W_B=ones(N2,N1);

 $W_Y=ones(N2,N1);$

EPS_S=ones(N2,N1);

EPS_B=ones(N2,N1);

EPS_Y=ones(N2,N1);

RHO_Y12=zeros(N2,N1);

MASS=ones(N2,N1);

M=ones(N2,N1);

%3.Transport Parameters

M100=zeros(N2,N1);

RHO_TRUE=zeros(N2,N1);

RHO_BULK=zeros(N2,N1);

CP_MASS=zeros(N2,N1);

K_MASS=zeros(N2,N1);

TK=zeros(N2,N1);

D_EFF=zeros(N2,N1);

RHO_AIR=zeros(N2,N1);

RHO_VAP=zeros(N2,N1);

RHO_Y=zeros(N2,N1);

RHO_WAT=zeros(N2,N1);

RHO_12=zeros(N2,N1);

CP_AIR=zeros(N2,N1);

CP_VAP=zeros(N2,N1);

CP_WAT=zeros(N2,N1);

MU_AIR=zeros(N2,N1);

MU_VAP=zeros(N2,N1);

MU_WAT=zeros(N2,N1);

K_AIR=zeros(N2,N1);

K_VAP=zeros(N2,N1);

K_WAT=zeros(N2,N1);

ENT=zeros(N2,N1);

PORE=zeros(N2,N1);

PERM_AIR=zeros(N2,N1);

PERM_WAT=zeros(N2,N1);

SURF=zeros(N2,N1);

XI=zeros(N2,N1);

K_EFF=zeros(N2,N1);

RHO=zeros(N2,N1);

C=zeros(N2,N1);

F0=zeros(N2,N1);

PR_B=zeros(N2,N1);

PR_Y=zeros(N2,N1);

SC=zeros(N2,N1);

P_1=zeros(N2,N1);

P_2=zeros(N2,N1);

P_Y=zeros(N2,N1);

- SU=zeros(N2,N1);
- AN=zeros(N2,N1);
- AT=zeros(N2,N1);
- AS=zeros(N2,N1);
- AB=zeros(N2,N1);
- APO=zeros(N2,N1);
- AP=zeros(N2,N1);
- P_R=zeros(N2,N1);
- P_Z=zeros(N2,N1);
- RHO_1=zeros(N2,N1);
- RHO_2=zeros(N2,N1);
- T_R1=zeros(N2,N1);
- T_Z1=zeros(N2,N1);
- DELTA1=zeros(N2,N1);
- DELTA2=zeros(N2,N1);
- T_test=zeros(KTOTAL+1,1);
- time_test=zeros(KTOTAL+1,1);
- MC_test=zeros(KTOTAL+1,1);
- m_test=zeros(KTOTAL+1,1);

 $W_Y(1,:)=W_Y0;$

W_Y(2:end,:)=0;

EPS_Y(2:end,:)=0.01;

EPS_B(1,:)=0;

 $M(:,:)=M_0;$

RHO_Y12(:,:)=0.00001;

```
T_test(1)=T_0;
```

m_test(1)=.1;

time_test(1)=0;

```
MC_test(1)=100*M_0;
```

```
for J=1:N1;
```

```
for I=1:N2;
%Initial Properties
%A. Coffee Mass Density (1-4) - Perez-Alegria (2001)
```

%Correlations taken from Perez-Alegria (2001) use M.C.(%w.b.) M100(I,J)=100*M(I,J); %100*(M(I,J)/(1+M(I,J)));

RHO_TRUE(I,J)=P(1)*M100(I,J)+P(2); %kg/m3

RHO_BULK(I,J)=P(3)*M100(I,J)+P(4); %kg/m3

%B. Coffee Mass Specific Heat (5-6) - Perez-Alegria (2001) CP_MASS(I,J)=P(5)*M100(I,J)+P(6); %kJ/kg-K

```
%C. Coffee Mass Effective Thermal Conductivity (7-8) - Perez-Alegria (2001)
```

```
K_MASS(I,J)=P(7)*M100(I,J)+P(8); %W/m-K
```

%D. Coffee Mass Total Effective Diffusivity (9-11) - Correa (2006)

TK(I,J)=T(I,J)+273.15;

D_EFF(I,J)=P(9)*exp(P(10)/(P(11)*TK(I,J))); %m2/s

- %****All fluid properties correlated herein were evaluated in Celsius
 degrees
- %E. Dry Air Density (12-17)
- RHO_AIR(I,J)=P(12)+P(13)*T(I,J)+P(14)*T(I,J)^2+P(15)*T(I,J)^3+ ... P(16)*T(I,J)^4+P(17)*T(I,J)^5; %kg/m3
- %F. Water Vapor Density (18-23)
- RHO_VAP(I,J)=P(18)+P(19)*T(I,J)+P(20)*T(I,J)^2+P(21)*T(I,J)^3+ ... P(22)*T(I,J)^4+P(23)*T(I,J)^5; %kg/m3
- %G. Moist Air density
- RHO_Y(I,J)=RHO_AIR(I,J)+RHO_VAP(I,J);
- %H. Liquid Water Density (24-29)
- RHO_WAT(I,J)=P(24)+P(25)*T(I,J)+P(26)*T(I,J)^2+P(27)*T(I,J)^3+ ... P(28)*T(I,J)^4+P(29)*T(I,J)^5; %kg/m3
- %I. Dry Air Specific Heat (30-35)
- CP_AIR(I,J)=(P(30)+P(31)*T(I,J)+P(32)*T(I,J)^2+P(33)*T(I,J)^3+ ... P(34)*T(I,J)^4+P(35)*T(I,J)^5)*1000; %J/kg-K
- %J. Water Vapor Specific Heat (36-41)
- CP_VAP(I,J)=(P(36)+P(37)*T(I,J)+P(38)*T(I,J)^2+P(39)*T(I,J)^3+ ... P(40)*T(I,J)^4+P(41)*T(I,J)^5)*1000; %J/kg-K
- %K. Liquid Water Specific Heat (42-47)
- CP_WAT(I,J)=P(42)+P(43)*T(I,J)+P(44)*T(I,J)^2+P(45)*T(I,J)^3+ ... P(46)*T(I,J)^4+P(47)*T(I,J)^5; %J/kg-K
- %L. Dry Air Dynamic Viscosity (48-53)

MU_AIR(I,J)=(P(48)+P(49)*T(I,J)+P(50)*T(I,J)^2+P(51)*T(I,J)^3+ ...

P(52)*T(I,J)^4+P(53)*T(I,J)^5)/1000000; %kg/m-s

- %M. Water Vapor Dynamic Viscosity (54-59)
- MU_VAP(I,J)=(P(54)+P(55)*T(I,J)+P(56)*T(I,J)^2+P(57)*T(I,J)^3+ ... P(58)*T(I,J)^4+P(59)*T(I,J)^5)/10000000; %kg/m-s
- %N. Liquid Water Dynamic Viscosity (60-65)
- MU_WAT(I,J)=(P(60)+P(61)*T(I,J)+P(62)*T(I,J)^2+P(63)*T(I,J)^3+ ... P(64)*T(I,J)^4+P(65)*T(I,J)^5)/1000; %kg/m-s
- %~N. Dry Air Thermal Conductivity (66-71)
- K_AIR(I,J)=P(66)+P(67)*T(I,J)+P(68)*T(I,J)^2+P(69)*T(I,J)^3+ ... P(70)*T(I,J)^4+P(71)*T(I,J)^5; %W/m-K
- %O. Water Vapor Thermal Conductivity (72-77)

K_VAP(I,J)=(P(72)+P(73)*T(I,J)+P(74)*T(I,J)^2+P(75)*T(I,J)^3+ ... P(76)*T(I,J)^4+P(77)*T(I,J)^5)/1000; %W/m-K

- %P. Liquid Water Thermal Conductivity (78-83)
- K_WAT(I,J)=(P(78)+P(79)*T(I,J)+P(80)*T(I,J)^2+P(81)*T(I,J)^3+ ... P(82)*T(I,J)^4+P(83)*T(I,J)^5)/100; %W/m-K

%Q. Latent Heat of Vaporization - Cengel (84-87)

ENT(I,J)=(P(84)+P(85)*T(I,J)+P(86)*T(I,J)^2+P(87)*T(I,J)^3)*1000;

%kJ/kg

%R. Permeability (88-90) -----

PERM_BEAN=P(88); %Single bean permeability determined by Ocasio (2014)

```
PORE(I,J)=1-(RHO_BULK(I,J)/RHO_TRUE(I,J)); %Porosity
```

EPS_S(I,J)=1-PORE(I,J);

```
TAU=(PORE(I,J)^2)/(8*P(89)^2);
```

PERM_BED=TAU*P(90)/(10000);

PERM_AIR(I,J)=PORE(I,J)*PERM_BED+(1-PORE(I,J))*PERM_BEAN; %m^2

PERM_WAT(I,J)=PERM_BEAN; %m^2

```
%S. Surface Tension (91-94)
```

```
SURF(I,J)=P(91)*(((P(92)-TK(I,J))/P(92))^P(93))*(1+P(94)* ...
(P(92)-TK(I,J))/P(92)); %N/m
```

%T. Radius of Interface Curvature (93)

R_CURV=P(95); %m

%U. Gases Specific Constants

R_AIR=R_IDEAL/MAIR;

R_VAP=R_IDEAL/MH2O;

%V. Liquid Volume Fraction IC

EPS_B(2:end,:)=PORE(2,1);

%W. Intrinsic Phase Gas Density
RH0_Y12(1,:)=RH0_AIR(1,1);

%X. Liquid Phase Discontinuities Parameter (M.Ocasio [2015])

XI(I,J)=EPS_B(I,J)/PORE(I,J);

end

_ _ _ _ _ _

end

%% TIME LOOP

for K=1:KTOTAL;

%% IV. OLD TRANSPORT QUANTITIES

T0=T;

W_Y0=W_Y;

 $W_B0=W_B;$

U_Y0=U_Y;

U_B0=U_B;

RHO_WATO=RHO_WAT;

RH0_01=RH0_1;

EPS_B0=EPS_B;

EPS_Y0=EPS_Y;

C_0=C;

CP_0VAP=CP_VAP;

CP_OWAT=CP_WAT;

ENT_0=ENT;

RH0_Y012=RH0_Y12;

%Local Time

```
TIME=DTIME*K/3600;
```

TIMEs=DTIME*K;

```
fprintf('Time= %.f s M.C.(w.b.)=%.5f m_dot=%.5f kg/(s*m3) \n',TIMEs-
DTIME,100*M(1,1),mean(mean(MASS)));
```

%Supply Air

T_S=T_SA(1)+T_SA(2)*TIME+T_SA(3)*TIME^2+ ... T_SA(4)*TIME^3+T_SA(5)*TIME^4+T_SA(6)*TIME^5+ ... T_SA(7)*TIME^6+T_SA(8)*TIME^7+T_SA(9)*TIME^8+ ... T_SA(10)*TIME^9; %Air Inlet Temperature (Celsius)

T(1,:)=T_S;

%% V. PROPERTIES

for Q=1:ITER;

	for J=1:N1;		
		for	I=1:N2;
			%A. Coffee Mass Density (1-4) - Perez-Alegria (2001)
			%Correlations taken from Perez-Alegria (2001) use M.C.(%w.b.)
			M100(I,J)=100*M(I,J); %100*(M(I,J)/(1+M(I,J)));
			RHO_TRUE(I,J)=P(1)*M100(I,J)+P(2); %kg/m3
			RHO_BULK(I,J)=P(3)*M100(I,J)+P(4); %kg/m3
			<pre>%B. Coffee Mass Specific Heat (5-6) - Perez-Alegria (2001)</pre>
			CP_MASS(I,J)=P(5)*M100(I,J)+P(6); %kJ/kg-K
			<pre>%C. Coffee Mass Effective Thermal Conductivity (7-8) - Perez- Alegria (2001)</pre>
(2006)			<pre>K_MASS(I,J)=P(7)*M100(I,J)+P(8); %W/m-K</pre>
			%D. Coffee Mass Total Effective Diffusivity (9-11) - Correa
			TK(I,J)=T(I,J)+273.15;
			<pre>D_EFF(I,J)=P(9)*exp(P(10)/(P(11)*TK(I,J))); %m2/s</pre>
			<pre>%****All fluid properties correlated herein were evaluated in Celsius degrees</pre>
			%E. Dry Air Density (12-17)
			RHO_AIR(I,J)=P(12)+P(13)*T(I,J)+P(14)*T(I,J)^2+P(15)*T(I,J)^3+
			P(16)*T(I,J)^4+P(17)*T(I,J)^5; %kg/m3
			%F. Water Vapor Density (18-23)
			RHO_VAP(I,J)=P(18)+P(19)*T(I,J)+P(20)*T(I,J)^2+P(21)*T(I,J)^3+

	P(22)*T(I,J)^4+P(23)*T(I,J)^5; %kg/m3
	%G. Moist Air density
	<pre>RHO_Y(I,J)=RHO_AIR(I,J)+RHO_VAP(I,J);</pre>
	%H. Liquid Water Density (24-29)
	RHO_WAT(I,J)=P(24)+P(25)*T(I,J)+P(26)*T(I,J)^2+P(27)*T(I,J)^3+
•••	P(28)*T(I,J)^4+P(29)*T(I,J)^5; %kg/m3
	%I. Dry Air Specific Heat (30-35)
	CP_AIR(I,J)=(P(30)+P(31)*T(I,J)+P(32)*T(I,J)^2+P(33)*T(I,J)^3+
•••	P(34)*T(I,J)^4+P(35)*T(I,J)^5)*1000; %J/kg-K
	%J. Water Vapor Specific Heat (36-41)
	CP_VAP(I,J)=(P(36)+P(37)*T(I,J)+P(38)*T(I,J)^2+P(39)*T(I,J)^3+
•••	P(40)*T(I,J)^4+P(41)*T(I,J)^5)*1000; %J/kg-K
	%K. Liquid Water Specific Heat (42-47)
	CP_WAT(I,J)=P(42)+P(43)*T(I,J)+P(44)*T(I,J)^2+P(45)*T(I,J)^3+
•••	P(46)*T(I,J)^4+P(47)*T(I,J)^5; %J/kg-K
	%L. Dry Air Dynamic Viscosity (48-53)
	MU_AIR(I,J)=(P(48)+P(49)*T(I,J)+P(50)*T(I,J)^2+P(51)*T(I,J)^3+
•••	P(52)*T(I,J)^4+P(53)*T(I,J)^5)/1000000; %kg/m-s
	%M. Water Vapor Dynamic Viscosity (54-59)
	MU_VAP(I,J)=(P(54)+P(55)*T(I,J)+P(56)*T(I,J)^2+P(57)*T(I,J)^3+
	P(58)*T(I,J)^4+P(59)*T(I,J)^5)/10000000; %kg/m-s
	%N. Liquid Water Dynamic Viscosity (60-65)
	MU_WAT(I,J)=(P(60)+P(61)*T(I,J)+P(62)*T(I,J)^2+P(63)*T(I,J)^3+
	P(64)*T(I,J)^4+P(65)*T(I,J)^5)/1000; %kg/m-s

	%~N. Dry Air Thermal Conductivity (66-71)
	<pre>K_AIR(I,J)=P(66)+P(67)*T(I,J)+P(68)*T(I,J)^2+P(69)*T(I,J)^3+</pre>
•••	P(70)*T(I,J)^4+P(71)*T(I,J)^5; %W/m-K
	%O. Water Vapor Thermal Conductivity (72-77)
	K_VAP(I,J)=(P(72)+P(73)*T(I,J)+P(74)*T(I,J)^2+P(75)*T(I,J)^3+
•••	P(76)*T(I,J)^4+P(77)*T(I,J)^5)/1000; %W/m-K
	%P. Liquid Water Thermal Conductivity (78-83)
	K_WAT(I,J)=(P(78)+P(79)*T(I,J)+P(80)*T(I,J)^2+P(81)*T(I,J)^3+
•••	P(82)*T(I,J)^4+P(83)*T(I,J)^5)/100; %W/m-K

%Q. Latent Heat of Vaporization - Cengel (84-87)

```
ENT(I,J)=(P(84)+P(85)*T(I,J)
+P(86)*T(I,J)^2+P(87)*T(I,J)^3)*1000;
```

%kJ/kg

%S. Surface Tension (91-94)

SURF(I,J)=P(91)*(((P(92)-TK(I,J))/P(92))^P(93))*(1+P(94)* ...

(P(92)-TK(I,J))/P(92)); %N/m

%T. Radius of Interface Curvature (93)

R_CURV=P(95); %m

%T. Gases Specific Constants

R_AIR=R_IDEAL/MAIR;

R_VAP=R_IDEAL/MH2O;

%U. Liquid Phase Discontinuities Parameter (M.Ocasio [2014])

XI(I,J)=EPS_B(I,J)/PORE(I,J);

%According to [Withaker (1977), p.174] we must be careful to %choose the reference pressure p0 as the intrinsic phase average %pressure at point <r>=0 so that the term <p_y-p0>-rho_y*<r>*g is %zero under hydrostatic conditions. %Gas-phase pressure calculation (p_gamma-p_0) %NOTE: In the gas phase motion equation p_gamma represents the % total pressure; therefore, p_gamma=p_0+rho*g*r+p_dynamic. This implies that grad(p gamma-p 0-rho*g*r) is the % gradient % of the dynamic pressure, which leads us to calculate this % phase velocity using Navier-stokes quasi steady approximation % grad(p_dynamic)=viscosity*grad2(velocity). %V.Mass fraction weighted thermal conductivity K_EFF(I,J)=EPS_S(I,J)*K_MASS(I,J)+EPS_B(I,J)* ... K_WAT(I,J)+EPS_Y(I,J)*K_VAP(I,J);

%W.Average density (RHO)

RHO(I,J)=EPS_S(I,J)*RHO_TRUE(I,J)+EPS_B(I,J)*RHO_WAT(I,J)+ ... EPS_Y(I,J)*(RHO_AIR(I,J)+RHO_VAP(I,J));

%X.Mass fraction weighted averaged heat capacity

C(I,J)=(EPS_S(I,J)*RHO_TRUE(I,J)*CP_MASS(I,J)+ ... EPS_B(I,J)*RHO_WAT(I,J)*CP_WAT(I,J)+ ... EPS_Y(I,J)*(RHO_AIR(I,J)*CP_AIR(I,J)+ ... RHO_VAP(I,J)*CP_VAP(I,J))/RHO(I,J);

%At this moment the effective conductivity is evaluated as if %conduction heat transfer in air could be neglected

%Y.Reference Values

LC=R_CURV;

%LC=1.47E-002;

U_INF=W_Y(1,1);

RHO_INF=RHO_AIR(1,1);

TIME_C=LC/U_INF;

DT_MAX=(T_Smax-T_0);

%Z.Dimensionless Numbers

RE=(RHO_Y(1,1)*U_INF*LC)/MU_AIR(1,1);

FO(I,J)=K_EFF(I,J)*TIME_C/(RHO(I,J)*C(I,J)*LC);

PR_B(I,J)=CP_WAT(I,J)*MU_WAT(I,J)/K_WAT(I,J);

PR_Y(I,J)=(CP_AIR(I,J)*MU_AIR(I,J)/K_AIR(I,J)+... CP_VAP(I,J)*MU_VAP(I,J)/K_VAP(I,J))/2;

SC(I,J)=MU_VAP(I,J)/(RHO_VAP(I,J)*D_EFF(I,J));

%AA.Vaporization Rate

DELTA1(I,J)=(EPS_S(I,J)/PORE(I,J))*(ENT(I,J)-ENT_0(I,J))/

(DTIME);

DELTA2(I,J)=CP_WAT(I,J)*(T(I,J)+273.15)- ...
CP_OWAT(I,J)*(T0(I,J)+273.15);

if DELTA1(I,J)==0;

MASS(I,J)=0.1;

else

MASS(I,J)=DELTA1(I,J)/DELTA2(I,J);

end

end

end

%% VI. DIMENSIONLESS TRANSPORT QUANTITIES

Td=T/DT_MAX;

T0d=T0/DT_MAX;

U_Bd=U_B/U_INF;

U_Yd=U_Y/U_INF;

W_Bd=W_B/U_INF;

W_Yd=W_Y/U_INF;

RHOd=RHO/RHO_INF;

RHO_Y12d=RHO_Y12/RHO_INF;

RHO_Y012d=RHO_Y012/RHO_INF;

RHO_Bd=RHO_WAT/RHO_INF;

DTd=DTIME/TIME_C;

%% VII. TOTAL ENERGY EQUATION

%Calculating matrix coefficients

for J=2:N1-1;

for I=2:N2-1;

R=J*DRd;

%Finite volume transfer areas

%Cylindrical coordinates

A_TB=2*R*DRd; %A_B=A_T A_N=(R+.5*DRd)*DZd;

A_S=(R-.5*DRd)*DZd;

%Diffusion Conductances

%Cylindrical coordinates

DN=((R+DRd))/((R+.5*DRd)*DRd); DNP=(R)/((R+.5*DRd)*DRd); DS=((R-DRd))/((R-.5*DRd)*DRd); DSP=(R)/((R-.5*DRd)*DRd); DT=1/DZd; DB=1/DZd; %Convention: T is the usual N, B is the usual S, %----- N is the usual E, S is the usual W

FT=0;

FB=0;

```
FN=0;
```

FS=0;

%Dimensionless cell Peclet number (Pe)

PET=FT/DT;

PEB=FB/DB;

PEN=FN/DN;

PES=FS/DS;

%Hybrid scheme functionS (+ eta and - eta)

%Тор

if PET<=2

PETA_T=0;

else

PETA_T=1;

end

if PET >= -2

NETA_T=0;

else

NETA_T=1;

end

%Bottom

if PEB<=2

PETA_B=0;

else

PETA_B=1;

end

if PEB>=-2

NETA_B=0;

else

NETA_B=1;

end

%North

if PEN<=2

PETA_N=0;

else

PETA_N=1;

end

if PEN>=-2

NETA_N=0;

else

NETA_N=1;

end

%South

if PES<=2

PETA_S=0;

else

PETA_S=1;

if PES>=-2

NETA_S=0;

else

NETA_S=1;

end

%Matrix coefficients

%1) Source Term (SU)

%Differential volume (DV)

DV=0.5*((R)^2-(R-DRd)^2)*DZd; %Cylindrical

%Source term

SU(I,J)=-(MASS(I,J)*LC^2/K_EFF(I,J))*(ENT(I,J)/DT_MAX)*DV... -((1/FO(I,J))*(RHOd(I,J)*DV*TOd(I,J))/DTd);

%MASS == volumetric vaporization rate ([M]/([T]*[L^3]))

%North Coefficient (AN)

NN(1)=-FN; NN(2)=(DN-0.5*FN); NN(3)=0; AN(I,J)=max(NN); %Top Coefficient (AT)

TT(1)=-FT; TT(2)=(DT-0.5*FT); TT(3)=0; AT(I,J)=max(TT);

%South Coefficient (AS)

SS(1)=FS; SS(2)=(DS+0.5*FS); SS(3)=0; AS(I,J)=max(SS);

%Bottom Coefficient (AB)

DF=FN-FS+FT-FB;

```
AP(I,J)=-(AN(I,J)+AT(I,J)+AS(I,J)+AB(I,J)+APO(I,J)+DF);
```

end

%Energy Equation Boundary Conditions

AP(1,:)=1; %Hot Surface

SU(1,:)=Td(1,:);

AP(2:end,1)=1; %R=0 wall (symmetry)

AN(2:end,1)=-1;

AP(2:end,N1)=1; %R=Rmax wall (symmetry)

AS(2:end,N1)=-1;

AP(N2,:)=1; %Z=Zmax (symmetry)

AB(N2,:)=-1;

KK=0;

```
A_TEMP=zeros(N3,5);
```

for I=1:N2;

for J=1:N1;

KK=KK+1;

 $A_{TEMP}(KK,:)=[AB(I,J) AS(I,J) AP(I,J) AN(I,J) AT(I,J)];$

end

end

%Sparse from Pentadiagonals

```
A_TEMP=spdiags(A_TEMP,D5,N3,N3);
A_TEMP=full(A_TEMP');
X=Td';
```

```
X=reshape(X,[N3,1]);
Y=SU';
Y=reshape(Y,[N3,1]);
[X,flag]=bicgstab(A_TEMP,Y,[],1500,[],[],X);
X=reshape(X,[N2,N1]);
Td=X';
```

%Boundary Conditions

Td(:,1)=Td(:,2); %R=0

Td(:,N1)=Td(:,N1-1); %R=Rmax

Td(N2,:)=Td(N2-1,:); %Z=Zmax

%Real Temperature Calculations
T=Td*DT_MAX;
%% VIII. PRESSURE
%RH and Sat Pressure Files
A1=A(1);

B1=A(2); C1=A(3); A2=A(4); B2=A(5); C2=A(6); %------

I1=II(1);
I2=II(2);

I3=II(3);

I4=II(4);

I5=II(5);

I6=II(6);

%-----01=0(1); 02=0(2);

03=0(3);

04=0(4);

05=0(5);

06=0(6);

%Calculations

ACC1=0; ACC2=0; for J=1,N1; I=1; ACC1=ACC1+T(I,J); I=N2; ACC1=ACC1+T(I,J); end TAVEI=ACC1/N1+273.15; TAVE0=ACC2/N2+273.15; _____

```
PSI=(A1*exp(-(((TAVEI-B1)/C1))^2) + A2*exp(-(((TAVEI-B2)/C2))^2))*1000;
```

```
PSO=(A1*exp(-(((TAVEO-B1)/C1))^2) + A2*exp(-(((TAVEO-B2)/C2))^2))*1000;
```

RHIexp=I1+I2*TIME+I3*TIME^2+I4*TIME^3+I5*TIME^4+I6*TIME^5;

RHOexp=01+02*TIME+03*TIME^2+04*TIME^3+05*TIME^4+06*TIME^5;

```
DP=.01*RHOexp*PSO-.01*RHIexp*PSI;
```

for I=1:N2

for J=1:N1

P_1(I,J)=PSI+I*(DP/(N2)); %Vapor Pressure Pa (N/m^2)

end

end

%% IX. GAS MOTION

%Internal

Nodes-----

for J=2:N1-1;

for I=2:N2-1;

P_R(I,J)=(0.5*(P_Y(I,J+1)+P_Y(I,J))- ... 0.5*(P_Y(I,J)+P_Y(I,J-1)))/DR;

 $P_Z(I,J)=(0.5^*(P_Y(I+1,J)+P_Y(I,J))- \dots \\ 0.5^*(P_Y(I,J)+P_Y(I-1,J)))/DZ;$

end

```
%Top Surface (Pressure Relief)
for J=2:N1-1;
    I=N2;
    P_R(I,J)=P_R(I-1,J);
    P_Z(I,J)=P_Z(I-1,J);
    end
    %
%Central Differences (gas dynamic pressure; relative)
%At this moment the reference pressure P_SA is assumed to
%be constant or uniform at the air inlet, therefore, the
%gradient of PO is 0. This will not be entirely true, since
%there's some back-pressure at the air inlet generated by the
%coffee mass bed physical resistance.
for J=2:N1-1;
```

for I=2:N2-1;

%Porous Media Flow Parameter (OMEGA)

OMEGA_Y=-PERM_AIR(I,J)*EPS_Y(I,J)/(MU_AIR(I,J));

%Gas phase velocity in the radial direction

U_Y(I,J)=OMEGA_Y*P_R(I,J);

notes

%Gas phase velocity in the vertical direction (*in the this was define as V instead of W)

W_Y(I,J)=OMEGA_Y*((P_Z(I,J))-(RHO_AIR(I,J)+ ...

end

%Gas Motion Boundary Conditions
W_Y(2:end,1)=0;
W_Y(2:end,end)=0;
W_Y(end,1:end)=W_Y(end-1,1:end);

%% X. LIQUID MOTION
T_REF=647.15;
P1=235.8E-2;
P2=1.256;
P3=-0.625;

%Central Differences

%Internal Nodes

for J=2:N1-1;

for I=2:N2-1;

T_R1(I,J)=(T(I,J)-(T(I,J)+T(I,J-1)))/DR; T_Z1(I,J)=(T(I,J)-T(I-1,J))/DZ;

end

end

%Bottom Surface

for J=2:N1-1;

I=1;

T_R1(I,J)=(0.5*(T(I,J+1)+T(I,J))-0.5*(T(I,J)+T(I,J-1)))/DR; T_Z1(I,J)=(T(I+1,J)-T(I,J))/DZ;

end

%Top Surface

for J=2:N1-1; I=N2;

T_R1(I,J)=(0.5*(T(I,J+1)+T(I,J))-0.5*(T(I,J)+T(I,J-1)))/DR; T_Z1(I,J)=(T(I,J)-T(I-1,J))/DZ;

end

%*The _X1 symbol is read as "first derivative with respect to X" $\,$

for J=2:N1-1;
 for I=1:N2;

%Surface tension differential

SURF T1=P1*P2*(((T REF-T(I,J))/T REF)^(P2-1))*(-1/T REF)* • • • (1+P3*((T_REF-T(I,J))/T_REF))+ ... P1*(((T_REF-T(I,J))/T_REF)^(P2))*(-P3/T_REF); %Porous Media Flow Parameter (OMEGA) ------OMEGA_B=-(4/R_CURV)*(EPS_B(I,J)*XI(I,J)*PERM_WAT(I,J))/ . . . (MU_WAT(I,J)); %Liquid phase velocity in the radial direction -----U_B(I,J)=OMEGA_B*SURF_T1*T_R1(I,J); %Liquid phase velocity in the vertical direction (*in the notes I may have referred to this as V instead of W) W_B(I,J)=OMEGA_B*SURF_T1*T_Z1(I,J); end

end

%% XII. LIQUID PHASE CONTINUITY (EPS_B CALCULATION)

AN(:,:)=0; AT(:,:)=0; AP(:,:)=0; AB(:,:)=0; AS(:,:)=0; for J=2:N1-1;
 for I=2:N2-1;
 R=(J-1)*DRd;

%Finite volume transfer areas

%Cylindrical coordinates

A_TB=0.5*((R+DRd)^2-(R-DRd)^2); A_N=(R+.5*DRd)*DZd; A_S=(R-.5*DRd)*DZd;

%Cylindrical coordinates

DN=0; DS=0; DT=0; DB=0;

%Convention: T is the usual N, B is the usual S, %----- N is the usual E, S is the usual W

%Convective mass flux per unit area

FT=0;

FB=0;

FN=0;

FS=0;

%Matrix coefficients

%1) Source Term (SU)

%Differential volume (DV)

DV=DRd*DZd; %Cylindrical

%Central differences (FLOWGRAD)

SU(I,J)=-(TIME_C/RHO_INF)*(MASS(I,J)/RHO_Bd(I,J))*DV-... (EPS_B0(I,J)*DV)/(DTd);

%North Coefficient (AN)

NN(1)=-FN; NN(2)=(DN-0.5*FN); NN(3)=0; AN(I,J)=max(NN);

%Top Coefficient (AT)

TT(1)=-FT; TT(2)=(DT-0.5*FT); TT(3)=0; AT(I,J)=max(TT);

%South Coefficient (AS)

SS(1)=FS; SS(2)=(DS+0.5*FS); SS(3)=0;

AS(I,J)=max(SS);

> BB(1)=FB; BB(2)=(DB+0.5*FB); BB(3)=0; AB(I,J)=max(BB);

%Central Coefficient (AP)

DF=FN-FS+FT-FB;

AP(I,J)=-(AN(I,J)+AT(I,J)+AS(I,J)+AB(I,J)+APO(I,J)+DF);

end

end

```
%Liquid Continuity Equation Boundary Conditions
AP(1,:)=1; %Hot Surface
SU(1,:)=EPS_B(1,:);
AP(2:end,1)=1; %R=0 wall (symmetry)
AN(2:N2-1,1)=-1;
SU(2:end,1)=0;
AP(2:end,N1)=1; %R=Rmax wall (symmetry)
```

```
AS(2:N2-1,N1)=-1;
```

SU(2:end,N1)=0;

AP(N2,:)=1; %Z=Zmax (symmetry)

AB(N2,:)=-1;

SU(N2,:)=0;

KK=0;

A_EPSB=zeros(N3,5);

for I=1:N2;

for J=1:N1;

KK=KK+1;

```
%Pentadiagonals builiding
```

 $A_EPSB(KK,:)=[AB(I,J) AS(I,J) AP(I,J) AN(I,J) AT(I,J)];$

end end

%Sparse from Pentadiagonals

A_EPSB=spdiags(A_EPSB,D5,N3,N3);

```
A_EPSB=full(A_EPSB');
```

X=EPS_B';

```
X=reshape(X,[N3,1]);
```

Y=SU';

Y=reshape(Y,[N3,1]);

for KK=1:N3;

X(KK)=Y(KK)/A_EPSB(KK,KK);

end

X=reshape(X,[N2,N1]);

EPS_B=X';

EPS_B(2:end,1)=EPS_B(2:end,2);

EPS_B(2:end,end)=EPS_B(2:end,end-1);

```
EPS_B(end,1:end)=EPS_B(end-1,1:end);
```

%% XIII. VOLUME FRACTIONS AND M.C.(%W.B.)

acc_mass1=0;

```
acc_mass2=0;
```

for J=1:N1;

for I=2:N2;

EPS_Y(I,J)=1-EPS_S(I,J)-EPS_B(I,J); acc_mass1=EPS_B(I,J)+acc_mass1; acc_mass2=EPS_S(I,J)+acc_mass2;

end

end

M(:,:)=M_0*(acc_mass1/(N1*N2-N1))/(1-acc_mass2/(N1*N2-N1));

```
AP(:,:)=0;
AB(:,:)=0;
AS(:,:)=0;
for J=2:N1-1;
for I=2:N2-1;
R=(J-1)*DRd;
%Finite volume transfer areas
%Cylindrical coordinates
A_TB=0.5*((R+DRd)^2-(R-DRd)^2);
A_N=(R+.5*DRd)*DZd;
A_S=(R-.5*DRd)*DZd;
```

%Cylindrical coordinates

DN=0; DS=0; DT=0; DB=0; %Convention: T is the usual N, B is the usual S, %----- N is the usual E, S is the usual W

%Convective mass flux per unit area

FT=0;

FB=0;

FN=0;

FS=0;

%Matrix coefficients

%1) Source Term (SU)

%Differential volume (DV)

DV=DRd*DZd; %Cylindrical

%Central differences (FLOWGRAD)

SU(I,J)=(TIME_C/RHO_INF)*MASS(I,J)*DV- ... (EPS_Y0(I,J)*RHO_Y012d(I,J)*DV)/(DTd);

%North Coefficient (AN)

NN(1)=-FN; NN(2)=(DN-0.5*FN); NN(3)=0; AN(I,J)=max(NN);

%Top Coefficient (AT)

TT(1)=-FT; TT(2)=(DT-0.5*FT); TT(3)=0; AT(I,J)=max(TT);

%South Coefficient (AS)

SS(1)=FS; SS(2)=(DS+0.5*FS); SS(3)=0; AS(I,J)=max(SS);

%Bottom Coefficient (AB)

BB(1)=FB; BB(2)=(DB+0.5*FB); BB(3)=0; AB(I,J)=max(BB);

%Central Coefficient (AP)

```
DF=FN-FS+FT-FB;
AP(I,J)=-(AN(I,J)+AT(I,J)+AS(I,J)+AB(I,J)+AP0(I,J)+DF);
```

end

end

%Gas Continuity Equation Boundary Conditions
AP(1,:)=1; %Hot Surface
SU(1,:)=RH0_Y12d(1,:);
AP(2:end,1)=1; %R=0 wall (symmetry)
AN(2:N2-1,1)=-1;

```
SU(2:end,1)=0;
```

AP(2:end,N1)=1; %R=Rmax wall (symmetry)

```
AS(2:N2-1,N1)=-1;
```

```
SU(2:end,N1)=0;
```

```
AP(N2,:)=1; %Z=Zmax (symmetry)
```

```
AB(N2,:)=-1;
```

```
SU(N2,:)=0;
```

KK=0;

```
A_RHOY=zeros(N3,5);
```

```
for I=1:N2;
```

for J=1:N1;

```
KK=KK+1;
```

```
A_RHOY(KK,:)=[AB(I,J) AS(I,J) AP(I,J) AN(I,J) AT(I,J)];
```

end

```
%Sparse from Pentadiagonals
```

```
A_RHOY=spdiags(A_RHOY,D5,N3,N3);
```

```
A_RHOY=full(A_RHOY');
```

X=RHO_Y12d';

```
X=reshape(X,[N3,1]);
```

Y=SU';

```
Y=reshape(Y,[N3,1]);
```

for KK=1:N3;

```
X(KK)=Y(KK)/A_RHOY(KK,KK);
```

```
X=reshape(X,[N2,N1]);
```

RH0_Y12d=X';

RHO_Y12d(2:end,1)=RHO_Y12d(2:end,2);

RHO_Y12d(2:end,end)=RHO_Y12d(2:end,end-1);

```
RH0_Y12d(end,1:end)=RH0_Y12d(end-1,1:end);
```

```
RHO_Y12=RHO_Y12d*RHO_INF;
```

```
%% XIII. PHASE DENSITIES AND PHASE PRESSURE
for J=1:N1;
```

```
for I=1:N2;
```

```
RHO_1(I,J)=P_1(I,J)/(R_VAP*TK(I,J));
RHO_2(I,J)=RHO_Y12(I,J)-RHO_1(I,J);
P_2(I,J)=RHO_2(I,J)*R_AIR*TK(I,J);
P_Y(I,J)=P_1(I,J)+P_2(I,J);
```

end

end

end

%%IX. OUTPUT FILES -----

T_test(K+1)=T(ceil(N2/2),ceil(N1/2));

time_test(K+1)=TIME;

```
m_test(K+1)=mean(mean(MASS));
```

```
MC_test(K+1)=100*mean(mean(M));
```

if K < 10

filename1 = ['CB1/FIELD/T_000' num2str(K) '.txt']; filename2 = ['CB1/FIELD/U_Y_000' num2str(K) '.txt']; filename3 = ['CB1/FIELD/W_Y_000' num2str(K) '.txt']; filename4 = ['CB1/FIELD/U_B_000' num2str(K) '.txt']; filename5 = ['CB1/FIELD/W_B_000' num2str(K) '.txt']; filename6 = ['CB1/FIELD/EPS_Y_000' num2str(K) '.txt']; filename7 = ['CB1/FIELD/EPS_B_000' num2str(K) '.txt']; filename8 = ['CB1/FIELD/MASS_000' num2str(K) '.txt']; filename9 = ['CB1/FIELD/RH0_Y12_000' num2str(K) '.txt']; elseif K >= 10 && K<100 filename1 = ['CB1/FIELD/T_00' num2str(K) '.txt']; filename2 = ['CB1/FIELD/U_Y_00' num2str(K) '.txt']; filename3 = ['CB1/FIELD/W_Y_00' num2str(K) '.txt']; filename4 = ['CB1/FIELD/U_B_00' num2str(K) '.txt']; filename5 = ['CB1/FIELD/W_B_00' num2str(K) '.txt']; filename6 = ['CB1/FIELD/EPS_Y_00' num2str(K) '.txt']; filename7 = ['CB1/FIELD/EPS_B_00' num2str(K) '.txt']; filename8 = ['CB1/FIELD/MASS_00' num2str(K) '.txt']; filename9 = ['CB1/FIELD/RH0_Y12_00' num2str(K) '.txt'];

elseif K >= 100

```
filename2 = ['CB1/FIELD/U_Y_0' num2str(K) '.txt'];
filename3 = ['CB1/FIELD/W_Y_0' num2str(K) '.txt'];
filename4 = ['CB1/FIELD/U_B_0' num2str(K) '.txt'];
filename5 = ['CB1/FIELD/W_B_0' num2str(K) '.txt'];
filename6 = ['CB1/FIELD/EPS_Y_0' num2str(K) '.txt'];
filename7 = ['CB1/FIELD/EPS_B_0' num2str(K) '.txt'];
filename8 = ['CB1/FIELD/MASS_0' num2str(K) '.txt'];
filename9 = ['CB1/FIELD/RH0_Y12_0' num2str(K) '.txt'];
```

%Writing the output text files

```
dlmwrite(filename1,T);
```

```
dlmwrite(filename2,U_Y);
```

dlmwrite(filename3,W_Y);

```
dlmwrite(filename4,U_B);
```

```
dlmwrite(filename5,W_B);
```

```
dlmwrite(filename6,EPS_Y);
```

```
dlmwrite(filename7,EPS_B);
```

```
dlmwrite(filename8,MASS);
```

```
dlmwrite(filename9,RH0_Y12);
```

end

```
R=zeros(N2,N1);
```

```
Z=zeros(N2,N1);
```

```
for J=1:N1;
    for I=1:N2;
```

```
R(I,J)=J*DR;
Z(I,J)=I*DZ;
```

end

```
dlmwrite('CB1/FIELD/R.txt',R);
dlmwrite('CB1/FIELD/Z.txt',Z);
dlmwrite('CB1/FIELD/TIME.txt',time_test);
dlmwrite('CB1/FIELD/m.txt',m_test);
dlmwrite('CB1/FIELD/MC.txt',MC_test);
dlmwrite('CB1/FIELD/T_test.txt',T_test);
dlmwrite('CB1/FIELD/TSTEP.txt',KTOTAL
```

Appendix II: Post-processing Code

%Statistical Analysis of Parchment Coffee Model for Heat and Mass Transf. %Research: Simultaneous Heat and Mass Transfer in the Dehydration % of Parchment Coffee C.Arabica % %Author: Moises Y. Ocasio

clear all close all clc close all hidden

% Changing directory to Experimental Data Directory

cd('/home/myobhel/Desktop/Research/MATLAB Code/CB1');

%% I. Plotting profiles

T=importdata('FIELD/T_test.txt');

MC=importdata('FIELD/MC.txt');

TIME=importdata('FIELD/TIME.txt');

MC_EXP=importdata('MOIST.txt');

T_EXP=importdata('MASS.txt');

plot(TIME,T,'bo',T_EXP(:,1),T_EXP(:,2),'bs',TIME,MC,'rd',MC_EXP(:,1),MC_EXP(:,
2),'rs');

```
title('Parchment Coffee Dehydration Dynamics
OB2','FontSize',17,'FontWeight','Bold');
```

```
xlabel('Time (hrs)', 'FontSize', 16);
```

```
h=legend('Mass Temp Model({^o}C)','Exp. Mass Temp({^o}C)','M.C.(%.w.b.)','Exp.
M.C.(%.w.b.)');
```

set(h, 'FontSize', 12)

set(gca, 'FontSize', 12, 'FontWeight', 'Bold')

ylim([20,70]);

xlim([0,9]);

grid on

saveas(gcf,'expcomp.png','png')

pause

%% II. Calculating Statistics

DTIME1=TIME(2)-TIME(1);

DTIME2=MC_EXP(2,1)-MC_EXP(1,1);

```
DTIME3=T_EXP(2,1)-T_EXP(1,1);
```

DT12=round(DTIME2/DTIME1);

DT13=round(DTIME1/DTIME3);

N=length(nonzeros(T));

M=length(T_EXP(:,1));

```
P=length(MC_EXP(:,1));
```

T=nonzeros(T);

```
MC=nonzeros(MC);
```

```
TIME(2:end)=nonzeros(TIME(2:end));
```

acc=0;

```
MC_NEW=zeros(P,1);
```

```
MC_NEW=MC_EXP(:,1);
```

```
for i=1:DT12:N;
```

acc=acc+1;

```
MC_NEW(acc)=MC(i);
```

end

```
acc2=0;
```

```
T_NEW=zeros(N,2);
```

```
T_NEW(:,2)=T;
```

for j=1:DT13:M;

acc2=acc2+1;

```
T_NEW(acc2,1)=T_EXP(j,1);
```

```
T_NEW(acc2,2)=T_EXP(j,2);
```

%% Calculating the percentage error

% Temperature error

e_T=zeros(N,1);

for i=1:N;

```
e_T(i)=100*abs(T_NEW(i,2)-T(i))/(.5*(T_NEW(i,2)+T(i)));
```

end

% M.C. error

e_M=zeros(P,1);

for j=1:P;

```
e_M(j)=100*abs(MC_EXP(j,2)-MC_NEW(j))/(0.5*(MC_EXP(j,2)+MC_NEW(j)));
```

end

%Calculating Frequencies

[REP1,error_T]=hist(e_T,5);

[REP2,error_M]=hist(e_M,5);

%Moisture Plots

subplot(2,1,1);

plot(MC_EXP(:,1),e_M,'bs-','MarkerSize',6)

xlim([0,9]);

grid on

```
title('M.C.(%w.b.) % of Difference - OB2', 'FontSize', 16, 'FontWeight', 'Bold');
```

xlabel('time (hrs)', 'FontSize', 15)

```
ylabel('% of difference', 'FontSize', 15)
subplot(2,1,2);
bar(error_M,REP2/N);
grid on
xlabel('% of difference', 'FontSize', 15)
ylabel('Relative Frequency', 'FontSize', 15)
saveas(gcf,'MC_error.png','png')
pause
%Temperature Plots
subplot(2,1,1);
plot(TIME,e_T,'bs-','MarkerSize',6)
grid on
title('Temperature % of Difference - OB2', 'FontSize', 16, 'FontWeight', 'Bold');
set(gca, 'FontSize', 12, 'FontWeight', 'Bold')
xlabel('time (hrs)', 'FontSize', 15)
ylabel('% of difference', 'FontSize', 15)
xlim([0,9])
subplot(2,1,2);
bar(error_T,REP1/N);
grid on
set(gca, 'FontSize', 12, 'FontWeight', 'Bold')
xlabel('% of difference', 'FontSize',15)
ylabel('Relative Frequency', 'FontSize', 15)
Te_ave=mean(e_T)
Te_std=std(e_T)
```

MCe_ave=mean(e_M)

MCe_std=std(e_M)

saveas(gcf,'T_error.png','png')