

Heat and mass transfer model for a coffee roasting process

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Abstract

The roasting of coffee is a complex process and it takes years of experience to be able to produce a quality cup of coffee (as well as consistently reproducing the same quality coffee). Although there are various factors that can influence the final taste of coffee, from the green bean processing method to the roasting equipment used, the most crucial part in coffee flavour development is the roasting process. Even the highest quality green coffee beans can be spoiled with improper roasting procedures. No set rules exist to produce a specific roast of coffee and roasting techniques differ from roaster to roaster. It is the objective of this study to model the roasting process for the purpose of system optimisation and control. The usefulness of the model to be implemented to predict the quality of the final roasted coffee (in other words the degree of roast) was also considered.

In order to model the roasting process, the heat and mass transfer that take place during roasting were investigated and further quantified by means of heat and mass transfer models. Three heat and mass transfer models were identified from literature to be able to adequately model the moisture content and temperature of the beans during roasting. From these models, the roasting process was modelled and the predicted roast profiles were obtained. For model validation, several experimental roasting procedures are conducted.

A comparison between the experimental and modelled results (for the 9.09 wt% green beans) showed that all three proposed models could predict the roast profiles fairly well, with some deviations occurring with prolonged roasting times. However, all three moisture loss models consistently overestimated the moisture loss that occurs during roasting, which improved somewhat for the longer roasting times. Two of the proposed models were found to be very sensitive for the higher initial moisture contents, where the predicted roast profiles showed higher overestimations than with the normal green coffee beans. The third model performed fairly similar with all initial moisture contents and no adverse reactions (such as the significant levels of overestimation seen with the other two models) to the increased moisture content could be observed. All three moisture loss models still showed a degree of overestimation of the moisture content during a roast.

The degree of roast of the roasted coffee beans was determined from the final moisture content, the roast loss percentage (which includes moisture loss, volatile release and dry matter) and the progression of the roast. It was found that some defining roasting characteristics of the coffee beans (referred to as the first and second crack) consistently occurred at the same temperatures, with the first crack occurring at about 175 to 180 °C, and the second crack occurring at temperatures above 200 °C. From this, it was concluded that a

rudimentary roast degree prediction can be made based on the progression of the roast and the final roast temperatures obtained.

It was finally concluded that all three models can be used in the optimisation and control of the coffee roasting process, although further investigation is needed into the optimisation of the moisture loss models. In conjunction with the end of roast temperatures, the predicted roast profiles could be used to give a simple prediction of the degree of roast. This could help to control the roasting process more effectively and assist in reproducing high-quality products.

Keywords: *Heat and mass transfer, modelling, coffee roasting, roast profile, degree of roast*

Opsomming

Warmte- en massa-oordrag model vir 'n koffie roosterproses

Die rooster van koffie is 'n komplekse proses en dit neem jare se ondervinding om in staat te wees om 'n kwaliteit koppie koffie te produseer (sowel as om dieselfde gehalte koffie herhalend te produseer). Alhoewel daar verskeie faktore is wat die finale smaak van koffie kan beïnvloed, van die groen boontjie prosesseringsmetode tot die roostertoerusting wat gebruik word, is die roosterproses die belangrikste deel in die ontwikkeling van die geur van die koffie. Selfs die beste gehalte groen koffiebone kan bederf word met onbehoorlike roosterprosesse. Daar bestaan nie vaste reëls om 'n spesifieke gehalte geroosterde koffie te produseer nie en die roostertegnieke verskil van rooster tot rooster. Die doel van hierdie studie is om die roosterproses vir die optimering en beheer van die stelsel te modelleer. Die moontlikheid om ook die gehalte van die finale geroosterde koffie met die geïmplementeerde model te voorspel, met ander woorde die graad van rooster, is ook oorweeg.

Met die oog op die modellering van die roosterproses is die warmte- en massa-oordrag, wat tydens die proses plaasvind, ondersoek en verder gekwantifiseer deur middel van warmte- en massa-oordrag modelle. Daar is drie warmte- en massa-oordrag modelle, wat voldoende is om die voginhoud en temperatuur van die bone gedurende die roosterproses te modelleer, uit die literatuur geïdentifiseer. Die roosterproses is met hierdie modelle gemodelleer en die voorspelde roosterprofile verkry. 'n Aantal eksperimentele roosterprosedures is vir modelvalidering uitgevoer.

'n Vergelyking tussen die eksperimentele en gemodelleerde resultate (vir die 9,09 %_(massa) voginhoud groenbone) het getoon dat al drie voorgestelde modelle die geroosterde profile redelik goed kon voorspel, met 'n paar afwykings wat met verlengde roostertye voorgekom het. Al drie vogverlies-modelle het die vogverlies tydens die roosterproses, herhalend oorskat, maar het effens verbeter met die langer roostertye. Twee van die voorgestelde modelle was baie sensitief vir die hoër aanvanklike voginhoud, terwyl die voorspelde roosterprofile hoër oorskattings getoon het as met die normale groen koffiebone.

Die derde model het redelik soortgelyk met al die aanvanklike voginhoude gewerk en geen nadelige reaksies (soos die beduidende vlakke van oorskatting wat met die ander twee modelle waargeneem is) is met die verhoogde voginhoud waargeneem nie. Al drie vogverlies-modelle het steeds 'n mate van oorskatting van die voginhoud tydens 'n roosterproses getoon.

Die roostergraad van die geroosterde koffiebone is uit die finale voginhoud, die roosterverliespersentasie (wat vogverlies, vrylating van vlugtige stowwe asook droë materiaal insluit) en die vordering van die roosterproses bepaal. Daar is gevind dat sommige

definieerbare roostereienskappe van die koffiebone (verwys na as die eerste en tweede knal) gereeld by dieselfde temperature plaasgevind het, met die eerste knal wat by 175 tot 180 °C plaasvind en die tweede knal wat by temperature bo 200 °C plaasvind. Hieruit is die gevolgtrekking gemaak dat 'n elementêre roostergraadvoorspelling gemaak kan word op grond van die verloop van die roosterproses en die finale roostertemperature.

Ten slotte is die gevolgtrekking gemaak dat al drie modelle gebruik kan word in die optimering en beheer van die koffie roosterproses, alhoewel verdere ondersoeke oor die optimering van die vogverlies-modelle nodig is. Die eindtemperatuur, tesame met die voorspelde roosterprofiel kan gebruik word om 'n eenvoudige voorspelling van die graad van rooster te maak. Dit kan meehelp om die roosterproses meer effektief te beheer asook om hoë gehalte produkte te verseker.

Sleutelwoorde: *warmte- en massa-oordrag, modellering, koffie rooster, roosterprofiel, graad van rooster*

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Nomenclature

Abbreviation	Description
d.b.	On a dry basis
CV	Control volume
w.b.	On a wet basis
wt%	Weight percentage

Acronyms	Description
HTST	High temperature/short time
LTLT	Low temperature/long time
L-REA	Lumped reaction engineering approach
MRE	Mean relative error
REA	Reaction engineering approach
RMSE	Root mean square error

Symbol	Description	Unit
A	Surface area	m ²
Ar	Arrhenius equation prefactor	W/kg
a	Longitudinal diameter	m
a_w	Water activity	-
Bi	Biot number	-
b	Equatorial diameter	m
C_p	Heat capacity	J/kg·K
c	Moisture concentration	mol/m ³
D	Moisture diffusivity	m ² /s
d	Equivalent sphere diameter	m
dr	Length of control volume	m
ΔE	Activation energy	J/mol
e	Thickness	m
G	Mass flow rate	kg/s
ΔH_v	Latent heat of vaporisation	J/kg
He	Amount of heat produced as roasting continues	J/kg

Nomenclature

H_{et}	Total amount of heat produced during roasting	J/kg
h	Heat transfer coefficient	W/m ² ·K
h_e	Effective heat transfer coefficient	W/m ² ·K
K	Roast profile constant	-
k	Mass transfer coefficient	m/s
km	Internal mass transfer coefficient	m/s
L	Characteristic length for moisture diffusion	m
m	Weight	kg
N	The number of observations	-
Nu	Nusselt number	-
Pr	Prandtl number	-
p	Vapour concentration	kg/m ³
Q	Rate of heat generation (mass unit)	W/kg
q	Heat generation (volume unit)	W/m ³
$\dot{q}$	Rate of heat generation (volume unit)	W/m ³ ·s
R	Gas law constant	J/mol·K
R^2	Coefficient of determination	-
Re	Reynolds number	-
Rm	Diffusion resistance	s/m ³
Rt	Thermal resistance	K/W
RH	Relative humidity	%
RL	Roast loss	wt%
r	Radius	m
S	Specific surface area	m ² /m ³
T	Temperature	K
t	Time	s
$\dot{V}$	Volumetric flow rate	m ³ /hr
V	Volume	m ³
v	Velocity	m/s
X	Moisture content	kg/kg
Y	Observation	-
Z	Path length of gas flow across a substance	m

Nomenclature

Greek Symbol	Description	Unit
α	Thermal diffusivity	m ² /s
Λ	Asymptotic slopes for average drying curves	-
λ	Thermal conductivity	W/m·K
μ	Viscosity	kg/m·s
ρ	Density	kg/m ³
Φ	Rate of heat flow	W

Subscripts	Description
<i>avg</i>	Indicate average
<i>b</i>	Indicate the roasted medium (coffee bean)
<i>c</i>	Indicate the centre
<i>d.b</i>	Indicate a dry basis estimation
<i>exp</i>	Indicate experimental values
<i>eq</i>	Indicate at equilibrium
<i>ev</i>	Indicate evaporation
<i>g</i>	Indicate the roasting gas (air)
<i>i</i>	Indicate inlet (or initial) conditions
<i>m</i>	Indicate the metal of the roaster
<i>o</i>	Indicate outlet (or final) conditions
<i>p</i>	Indicate the middle
<i>pre</i>	Indicate predicted values
<i>r</i>	Indicated exothermic reactions
<i>rp</i>	Indicate the roast profile
<i>s</i>	surface
<i>sat</i>	saturation
<i>v</i>	Indicates water vapour

CHAPTER 1 – Introduction

Overview

In Chapter 1, a broad outline of the contents of this research study will be reported. The motivation for investigating the coffee roasting process is provided, as well as a discussion on the modelling of a coffee roasting process. This will serve as the background and motivation for this investigation (Section 1.1). From this the aims and objectives of the research study are formulated and stated in Section 1.2. Finally, this chapter ends with an overview of this document, with the scope of the investigation provided in Section 1.3.

“As long as there was coffee in the world, how bad could things be?” – C. Clare

1.1 Background and motivation

The morning cup of coffee that millions of people enjoy around the world can seem quite inconsequential, however the amount of preparation, work and money required to make the perfect “Cup of Joe” is staggering. As a tradable commodity, coffee is exported to every part of the globe from over 70 countries, where more than 125 million people are dependent on it for their livelihood (Hoffmann, 2014; Moldvaer, 2014). In 2015, more than 9 million tonnes of coffee was consumed, worth an estimated value of US \$ 109.5 billion (International Coffee Organization, 2016a, 2016b).

Coffee beans come from the cherries that grow on coffee trees and are in fact the dried out seeds of the cherry. These seeds are more commonly referred to as green coffee beans, which has almost no flavour, especially none of the characteristic flavours associated with the hot coffee beverage (Rao, 2014). The attractive flavours and aromas attributed to the coffee beverage are obtained through the roasting of green coffee beans, which is done by exposing the beans to hot gases or surfaces (Eggers & Pietsch, 2001). Coffee roasting is a complex process due to the simultaneous heat and mass transfer that takes place, which greatly influences the colour, aroma and flavour of the final produced product. The complexity of the process stems from the fact that, along with moisture loss and volatile release, several physical and chemical changes (which includes hydrolysis, polymerization, reduction, oxidation and decarboxylation) can also be observed (Putranto & Chen, 2012).

The roasting process involves three successive stages, which includes drying, pyrolysis and cooling. The slow release of water and other volatile substances takes place during the drying stage, where the bean will change in colour from green to yellow. This is followed by pyrolysis reactions, resulting in significant changes to the bean’s chemical and physical properties (Franca *et al.*, 2005; Putranto & Chen, 2012). During this stage, the bean experiences a rapid rise in temperature due to the occurrence of exothermic reactions. Throughout these reactions CO₂ is generated which is partially retained within the bean’s cells, increasing the pressure within the bean causing the bean to expand in size (Schwartzberg, 2002). Large amounts of CO₂, along with some water and volatile substances, are released (with an audible cracking/popping sound) as the pressure within the bean becomes too great and the bean doubles in size while it becomes half as dense. During pyrolysis, hundreds of chemical reactions take place, including the Maillard reaction which causes the bean to turn brown due to sugar caramelisation (Franca *et al.*, 2005; Putranto & Chen, 2012; Rao, 2014). Throughout this stage, more than 800 aroma compounds can develop. Lastly, a cooling stage is necessary to avoid burning and over development of coffee aromas (Franca *et al.*, 2005; Rao, 2014).

The quality of a final cup of coffee is influenced by many different factors along the line from the seed to the cup. These include growing, harvesting, processing and storage methods of the green coffee beans as well as several factors during the roasting process (including roaster type, roasting time and temperature and conditions of the roasting gas). Of all these factors, the roasting process is the most crucial part, for even the highest grade of green coffee beans can be ruined with inadequate roasting (Hoffmann, 2014; Yeretzian *et al.*, 2012). The condition of the final roasted coffee bean, as influenced by the various roasting conditions, is described as the degree of roast. The degree of roast is often determined by several properties of the roasted coffee, i.e. colour development of the bean, weight loss during the roasting process (more commonly referred to as roast loss) and moisture content of the bean (Baggenstoss *et al.*, 2008; Wang & Lim, 2014). The degree of coffee roasting is generally categorised into light, medium and dark roasting, which is primarily connected to the observed colour development of the coffee beans during the roasting process (Wang & Lim, 2014).

Currently, there is no standardised procedure to obtain specific roast degrees, and various roasting conditions are adjusted during the roasting process to acquire a specific product quality and roast degree. The artisan roaster needs to continuously analyse the beans during the roasting process, due to the absence of sufficient control systems, and accordingly adjust the roasting conditions to attain the preferred roast degree (Putranto & Chen, 2012). Once the desired flavour profile is accomplished by the artisan roaster, it is their aim to produce a consistent roast thereafter by duplicating the exact same roasting procedure (Yeretzian *et al.*, 2012).

The roasting reactions that occur during the coffee roasting process are dependent on both the duration of these reactions and the reaction rate. Furthermore, the reaction rate can be described to be dependent on the roasting temperature and the concentration of the reactant. To acquire the desired reproducible product flavour (also referred to as organoleptic properties) a bean temperature-time history control strategy needs to be implemented during the entire roast cycle (Schwartzberg, 2002).

1.2 Focus of study

During commercial roasting, an artisan roaster will continuously evaluate the progression of the roast. The artisan roaster interprets the noticeable changes (such as bean colour, sound of first and second crack, and aroma formation) throughout the roast and compares it to the measured roast profile in order to determine necessary adjustments that should be made to achieve a specific end product quality (or degree of roast) (Hernández *et al.*, 2007; Putranto & Chen, 2012). No set rules exist to produce a specific roast, and it takes years of learning

and experience to be able to evaluate the roast and incorporate the correct adjustments to produce a superior quality product.

In order to acquire the best quality roasted coffee, an accurate real-time estimation and prediction model are required for the roasting process. From this, the optimum roasting procedure can be derived and further controlled to deliver a reproducible high-quality product. In order to obtain this model, the temperature and moisture development during the roasting process needs to be quantified and further related to the degree of roast. In recent years, many researchers have attempted to do this, by investigating the heat and mass transfer during the roasting of green coffee beans and proposing a model that can predict the temperature and moisture evolution within the beans. These researchers include: Basile & Kikic (2009), Burmester & Eggers (2010), Fabbri *et al.* (2011), Heyd *et al.* (2007), Putranto & Chen (2012) and Schwartzberg (2002).

Therefore the focus of this study is to investigate a model that can accurately predict the roasting process, which can be of use to optimise an ideal roast for the purpose of process control.

1.3 Aim and objectives

The purpose of this research is to investigate the mass and heat transfer of coffee beans during the roasting process, which will be done by investigating heat and mass transfer models for the roasting process. The data required to validate the proposed model for the coffee roasting process will be obtained from experimental runs conducted on a commercial roaster. The validated model can be useful in the development of a temperature control strategy for the coffee roasting process.

It will be the aim of this research project to achieve the following objectives:

- Investigate the heat and mass transfer models that can help to optimise the coffee roasting process, and to investigate whether the roast profile can be obtained from these models. The model will be validated by means of experimental roasts done on a commercial coffee roaster.
- Identify the degree of roast of the roasted coffee, by analysing weight loss during the roasting process (more commonly referred to as roast loss) and moisture content of the bean throughout the roast. From this, the stages of the roast profile will be linked to the degree of roast, which could further help with obtaining specific desired roasts.

1.4 Scope of investigation

This study is divided into six chapters, including this one, in order to accomplish the above-mentioned objectives. Figure 1.1 gives a brief schematic overview of the scope of this investigation. The content of each chapter is as follows:

In **Chapter 2** a complete literature review on the roasting of coffee is presented. The aim of this chapter is to obtain knowledge that will assist to complete this study. First, a brief background is given about the growing, harvesting and processing of green coffee beans. Followed by a detailed discussion about all aspects related to coffee roasting. These include the coffee bean behaviour during roasting, e.g. how roasting affects its temperature, moisture content and mass, as well as the physical and chemical changes that the bean experiences. Other aspects like heat and mass transfer that takes place during roasting, the stages of coffee roasting, all parameters that can influence the roasting and finally the classifications of roasted coffee beans receive attention in this section. Lastly, an in-depth look is taken at the research that has been conducted thus far on the subject of modelling of the roasting process. This will help determine the viability of the proposed models and whether or not these can be applied to achieve the above-mentioned objectives.

In **Chapter 3** the experimental methodology followed for the roasting experimental programme are described in detail. This includes a description of the green coffee beans used as well as all experimental apparatus and equipment used to facilitate the roasting experiments.

Chapter 4 focuses on the modelling of the roasting process. Here all relevant heat and mass transfer models are presented and explained in detail. All parameters and equations used during modelling are given as well as a description of how the models were implemented and simulated. The models simulated are verified through comparison with literature based results.

Chapter 5 focuses on the results obtained from the roasting experiments as well as from the simulated heat and mass transfer models. The main focus here is to validate the heat and mass transfer model with the experimental data obtained. This is done by comparing the moisture content simulated by the model with the moisture content acquired from the experiments conducted. The roast profiles obtained during roasting is used to validate the roast profiles simulated by the model. Lastly, the degree of roast is estimated from the experimental results obtained from the final roasted beans and associated with the roast profile, so that a degree of roast prediction can be made from typical roast profile data.

The final chapter, **Chapter 6**, summarises the conclusions drawn following the results that were obtained throughout this investigation. From this, recommendations and suggestions will originate to support future work.

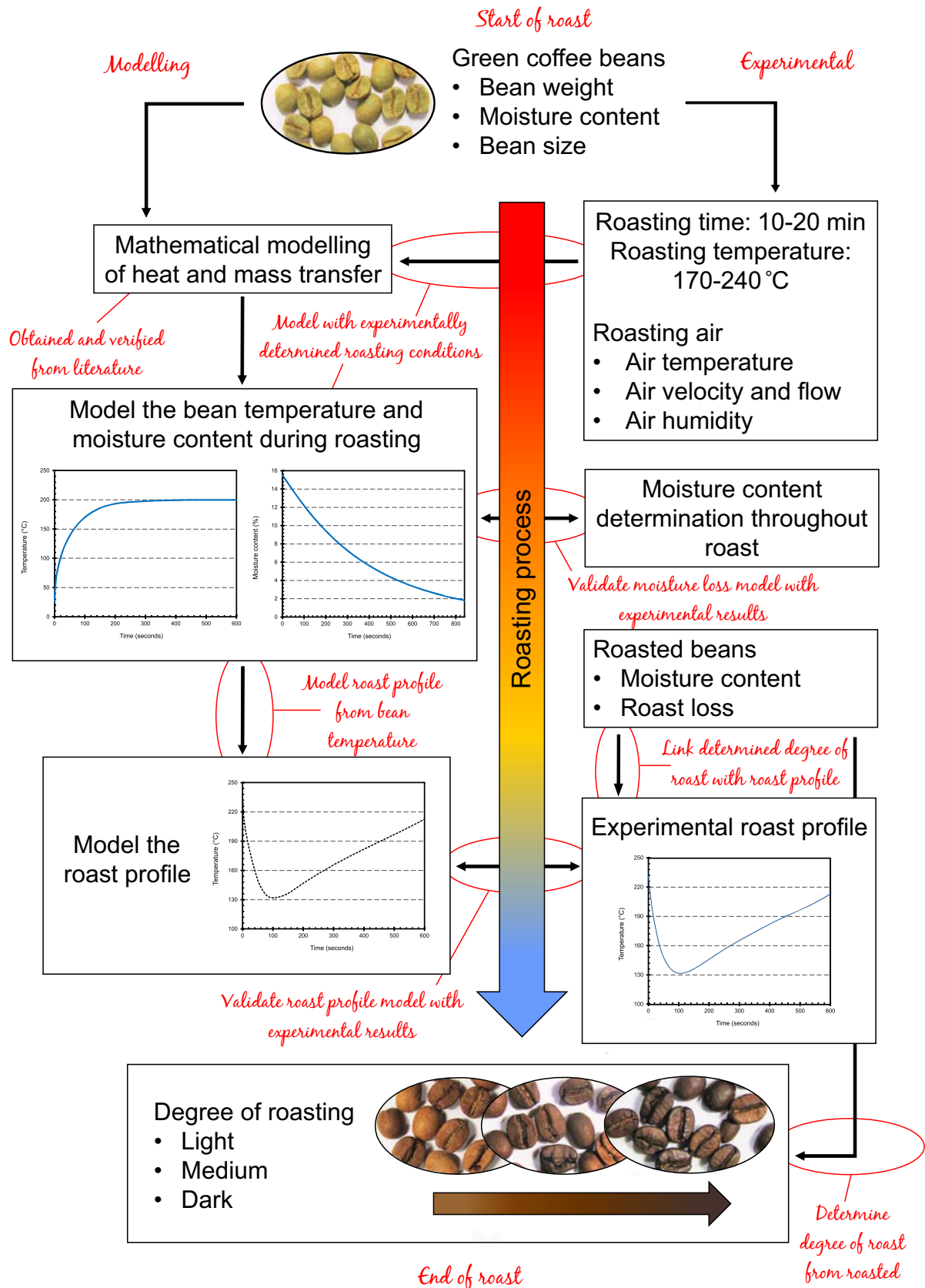


Figure 1.1: Schematic presentation of the scope of investigation

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CHAPTER 2: Literature review

Overview

In this chapter a complete literature review on the roasting of coffee is presented. The aim of this chapter is to obtain knowledge that will assist with model development. A brief background is given about green coffee beans in Section 2.1. This is followed by a detailed discussion on all aspects related to coffee roasting in Section 2.2, including bean behaviour during roasting, the heat and mass transfer that takes place, the five stages of coffee roasting and the classifications of roasted coffee beans. Section 2.3 is an in-depth discussion about the research that has been done thus far on the subject of modelling the roasting process. This will assist in determining the viability of the proposed models and whether or not these can be applied to achieve the objectives of this study.

"Even bad coffee is better than no coffee at all." – D. Lynch

2.1 The coffee bean

2.1.1 History of the coffee bean

Coffee was originally found in Ethiopia, Africa, however its use as a beverage spread from Arabia. Long before the coffee bean was roasted and crushed to be seeped in water, the coffee fruit was chewed for its invigorating properties. Travelling herders of Ethiopia would mix crushed dried coffee beans with fat and various spices to create a primitive form of the energy bar, that was used as sustenance when on long journeys (Moldvaer, 2014; Smith, 1985).

Around the 15th century, coffee was introduced into Arabia and Yemen; this is believed to have happened due to the spread of the slave trade. Soon the custom of steeping the ground roasted coffee beans to produce a beverage (much like how it is enjoyed today) spread throughout the Islamic world (Moldvaer, 2014; Smith, 1985). Initially, the consumption of coffee was banned by religious leaders, for it was believed to be an intoxicant. This led to the popularity of coffee houses being criticised as the main reason for poor attendance at the mosques (Smith, 1985).

By the 17th century it had spread all over Europe starting in Constantinople (modern-day Istanbul) and Venice, and by 1650 the first British coffee house opened in Oxford. Coffee's popularity grew fast and only 25 years later there were just about three thousand coffee houses in England (Belitz *et al.*, 2009; Smith, 1985). King Charles II quickly became suspicious of coffee houses assuming them to be the source of seditious gatherings and issued a decree that all coffee houses would be banned. This was hastily retracted due to strong opposition (and disapproval from the English people) and by the next century the coffee custom was well ingratiated into European and North American society (Smith, 1985).

The Arabians were the first to trade coffee, and as the only suppliers of coffee to the known world, they were very protective of their coffee beans, profoundly so that they boiled all their exported coffee beans to prevent anyone from trying to cultivate them (Moldvaer, 2014; Smith, 1985). However, early in the 17th century, coffee plants were smuggled from Yemen by a Dutch trader and was planted in Amsterdam. It was here the coffee beans were first classified as *Coffea Arabica* (most commonly referred to as Arabica) by the Amsterdam Botanical Gardens (Moldvaer, 2014; Smith, 1985).

In the late 19th century, Robusta was discovered in the Belgian Congo (modern-day Zaire) and was thusly named to highlight its qualities. This specific species was able to be cultivated at lower altitudes and in higher temperatures than the existing Arabica, as well as being more resilient against diseases (Hoffmann, 2014; Smith, 1985). These qualities were found to have great commercial potential for it could be produced at a significantly lower cost. However,

Robusta has one disadvantage: Arabica has a far superior taste. Yet today it is still widely produced around the world, for it is the main ingredient in instant soluble coffee (where the low production cost of the coffee far outweighs the perceived flavour) (Esquivel & Jimenez, 2012; Hoffmann, 2014).

Since its discovery, Robusta has been seen as inferior to Arabica, however a recent genetic discovery has shown that Robusta is, in fact, a parent of Arabica. It is believed that *Coffea eugenioides* (another coffee species) was crossed with Robusta in the southern region of Sudan to produce Arabica, from where it spread to Ethiopia. It was only in Ethiopia that it really began to flourish and be discovered (Hoffmann, 2014).

Of the 129 different known species of coffee only three are generally cultivated, namely *Coffea arabica* (which delivers roughly 60 % of the world's coffee production), *Coffea canephora* (about 40 % of the world's coffee production and most commonly referred to as Robusta) and *Coffea liberica* (less than 1 % of the world's production) (Belitz *et al.*, 2009; Hoffmann, 2014; International Coffee Organization, 2016a). Since its discovery, coffee has spread to all the corners of the world and is produced in more than 70 countries (Moldvaer, 2014). From Table 2.1 it can be seen that in the year 2015 almost 8.6 million tonnes of coffee were produced worldwide and that 88 % of the total world production comes from the top ten producing countries, with Brazil delivering 30 % of the world's coffee production. In the same year more than 9 million tonnes of coffee were consumed worldwide (International Coffee Organization, 2016b, 2016c).

Table 2.1: Production of coffee beans* in 2015 (adapted from International Coffee Organization, 2016b).

Continent	Raw coffee	Country	Raw coffee
World	8598	Brazil	2594
		Vietnam	1650
		Colombia	810
Africa	1047	Indonesia	739
Asia & Oceania	2868	Ethiopia	402
Central America	837	India	350
Europe	-	Honduras	345
North America	168	Uganda	285
South America	3678	Guatemala	204
		Peru	198
		Of world production	88%

*in 1000 tonne

2.1.2 The green coffee bean

Coffee beans come from the cherries that grow on coffee trees and are in fact the dried out seeds of the cherry. In each coffee fruit, there are two seeds that grow with their flat sides facing each other, as shown in Figure 2.1 (Moldvaer, 2014; Smith, 1985). In roughly 10 to 15 % of coffee fruits, only one seed develops and with nothing to flatten against, grows into an oval shaped bean known as a peaberry (Belitz *et al.*, 2009; Moldvaer, 2014).

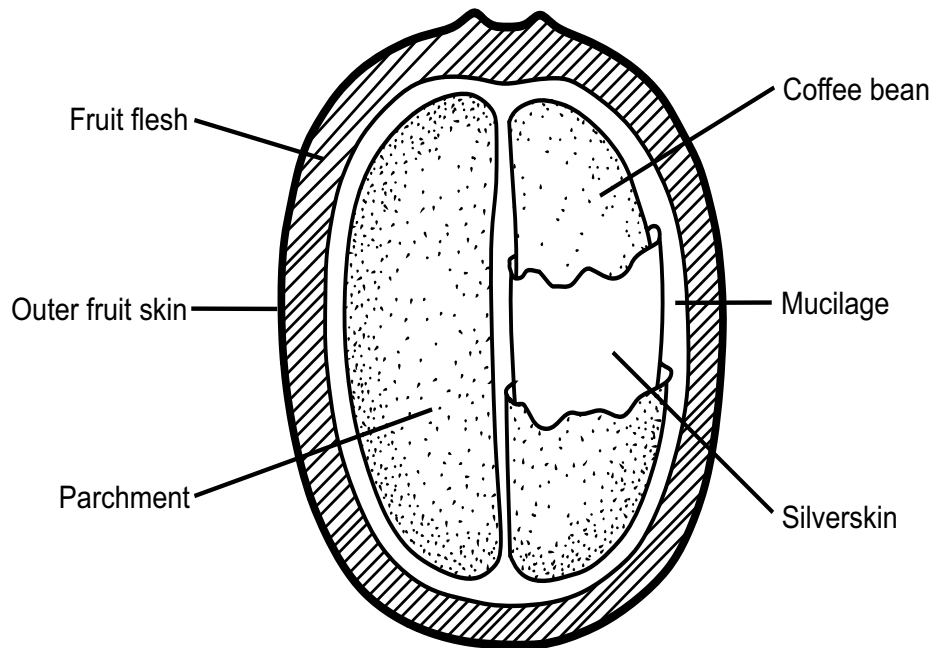


Figure 2.1: Layers of the coffee cherry (adapted from Belitz *et al.*, 2009).

The two seeds are both covered with a thin tightly fitted layer called the silverskin, followed by a yellowish looser skin known as the parchment. Both seeds are encased in a viscous and colourless mucilage layer, which is in turn surrounded by the fruit flesh or pulp. The coffee fruit has a tough outer skin that is green in colour, however it turns a deep red when ripe (Esquivel & Jimenez, 2012; Smith, 1985).

The composition of green coffee beans is highly dependent on various factors including climate, processing method, bean species and origin (Belitz *et al.*, 2009). On average about 50 % of the green coffee bean's composition is carbohydrates, where the other 50 % consists of water, lipids, alkaloids, proteins and acids. Since the method for determining the composition of green coffee beans is not a readily available procedure for coffee roasters, not much knowledge of this has to be known to produce a perfect roast batch of coffee (Rao, 2014).

2.1.3 Coffee harvesting

The coffee shrub is evergreen and can grow up to 12 meters in height depending on the species, however, to facilitate harvesting most shrubs are trimmed and kept at a height of 2 to 2.5 meters (Belitz *et al.*, 2009). About 4 years after planting, the shrub will start to bloom and will only provide a full harvest after 6 years; 12 months after flowering the coffee fruit will ripen, turning from green to a deep red, and be ready for harvest (Belitz *et al.*, 2009).

Several methods are utilised to harvest the coffee fruit, with some being more labour intensive than others. One method is to hand pick ripe coffee cherries from the tree, this ensures that only cherries ready for harvest is collected for processing (Belitz *et al.*, 2009; Moldvaer, 2014). Harvesting can also be done by strip picking, where entire branches are stripped when most of the cherries haven't ripened. This, however, can cause some immature cherries to be processed, influencing the quality of the final product. Other methods include mechanical harvesting and sweeping beneath the trees to collect the ripe cherries (Belitz *et al.*, 2009; Brando, 2004). Although harvesting is an important factor in the coffee production chain, any bad harvesting (harvesting producing a mixture of cherries in various stages of ripeness) can be minimised by the correct coffee processing method (Brando, 2004).

2.1.4 Coffee processing

The quality of the final cup of coffee can be influenced by many factors which include the green coffee processing method. Green coffee processing involves separating the fruit flesh from the bean as well as drying the beans for the purpose of safe storage (before drying, green coffee beans consist of about 60% moisture, afterwards it will contain less than 15%). This is done to ensure that it does not rot while in storage (Hoffmann, 2014; Rao, 2014).

For most coffee producers it is however not the final flavour that influences their chosen processing method but rather the effect processing has on the quality of their product and therefore the monetary value thereof (Hoffmann, 2014). Bad processing methods have been known to cause defects (a term used to describe an individual green coffee bean that developed problems during growing, harvesting and processing which resulted in bad flavours) giving the final brewed coffee a fermented taste. The three primary methods of processing are commonly referred to as the washed process, dry natural process and the pulped natural process (Hoffmann, 2014; Moldvaer, 2014; Rao, 2014).

2.1.4.1 Washed coffee processing

The washed coffee processing method is regarded as the more sophisticated processing method which generally leads to better quality coffee. This is due to the fact that the fruit flesh

is removed from the coffee bean before drying which significantly reduces the chance of something going wrong during the drying stage (Belitz *et al.*, 2009; Hoffmann, 2014).

The freshly harvested coffee cherries are first placed in a flotation tank where the ripe cherries separate from the unripe ones (the ripe cherries sink to the bottom while the unripe cherries float). The ripe cherries are then passed through a depulper where its outer skin and fruit flesh are stripped from the beans without damaging it. The pulped beans, which still have the silver skin, parchment and very sticky mucilage layers, are then carried to a water tank where the mucilage layer is removed by means of fermentation. This process takes up to 2 days. During this stage, the mucilage layer is degraded to such an extent that it can be washed off by water (Belitz *et al.*, 2009; Hoffmann, 2014; Rao, 2014).

After the removal of the mucilage layer, the coffee beans have a moisture content of about 50 % and is therefore in need of drying, by either mechanical driers or out in the sun. The dried product is known as parchment coffee and is stored in this condition until the time of exportation, where it goes through the final stages of processing which consist of cleaning, hulling (removing any remaining layers, including some of the silverskin) and grading (Hoffmann, 2014; Moldvaer, 2014; Vincent, 1987).

2.1.4.2 Dry natural coffee processing

The dry natural process is fairly straightforward and the more economical one of the three. Before the dry natural process can begin, the harvested cherries are sorted to remove any unripe fruit from processing. The ripe cherries are then dried in the sun for several weeks, after which it is stored awaiting exportation (Hoffmann, 2014; Smith, 1985). The dry natural process goes through the same final stages of the washed process mentioned above.

2.1.4.3 Pulped natural coffee processing

The pulped natural coffee processing method tends to produce sweeter coffee than the dry natural process. Just like with the washed process, the coffee cherries are placed in a flotation tank to remove the unripe cherries, after which the ripe cherries are passed through a depulper, removing the fruit flesh (Hoffmann, 2014; Rao, 2014). The coffee beans still encased in the silverskin, parchment and mucilage layer, are now set out to dry. The pulped beans dry fairly quickly, increasing its sweetness and body (this is due to being dried with the sugary mucilage layer). Just like with the above-mentioned processes, the dried pulped beans are stored until they undergo the final stages of processing and exportation (Hoffmann, 2014; Moldvaer, 2014; Rao, 2014).

2.2 Coffee roasting

2.2.1 Roasting process

The roasting of green coffee beans is required to develop the attractive flavours and aromas that can be found in a nice cup of coffee. Roasting is usually done by exposing the green beans to hot gases or surfaces which allows for the roasting reaction to take place, producing the hundreds of chemical compounds to which the aroma of brewed coffee is attributed (Eggers & Pietsch, 2001; Franca *et al.*, 2005).

Coffee roasting is complex due to the hundreds of reactions (which includes hydrolysis, polymerization, reduction, oxidation and decarboxylation) that takes place during the simultaneous heat and mass transfer within the coffee roaster. How the reactions take place and at what rates, greatly influences the colour, aroma and flavour of the final produced coffee product (Franca *et al.*, 2005; Putranto & Chen, 2012).

The entire roasting process can be divided into three steps: drying, roasting and cooling. The slow release of water and other volatile substances takes place during the drying step. This is followed by the roasting reactions, resulting in significant changes to the bean's chemical and physical properties, which is necessary for the aroma development. (Franca *et al.*, 2005; Putranto & Chen, 2012; Rao, 2014). When the coffee is roasted to the desired degree of roast, the coffee beans are immediately removed from the roasting chamber and the final step, the cooling phase, begins. The freshly roasted coffee is quickly cooled to prevent over roasting and to end exothermic reactions that occur within the beans at the later stages of roasting. Various cooling methods exist, however most commonly the beans are either sprayed with water (quenching) before it is removed from the roasting chamber or they are removed from the roaster and cooled with air (Baggenstoss *et al.*, 2000; Gloess *et al.*, 2014).

Figure 2.2 illustrates the basic concept of the heat and mass transfer that occurs during roasting. The basic coffee roasting process consists of heat transfer to the coffee bean by means of hot roasting air. This heat transfer initiates a rise in bean temperature which in return initiates several chemical and physical changes to occur. It is during these changes that the mass transfer takes place by the release of water vapour, CO₂ and volatiles, as well as the dry weight mass transfer that occurs (Eggers & Pietsch, 2001; Schwartzberg, 2002). During the roasting, exothermic reactions occur and heat is transfer from the bean to the surrounding environment (Schwartzberg, 2002). A more detailed description of the coffee roasting process will be discussed in the following sections, giving particular detail about the bean behaviour during roasting, the stages of coffee roasting and finally the classifications of roasted coffee beans.

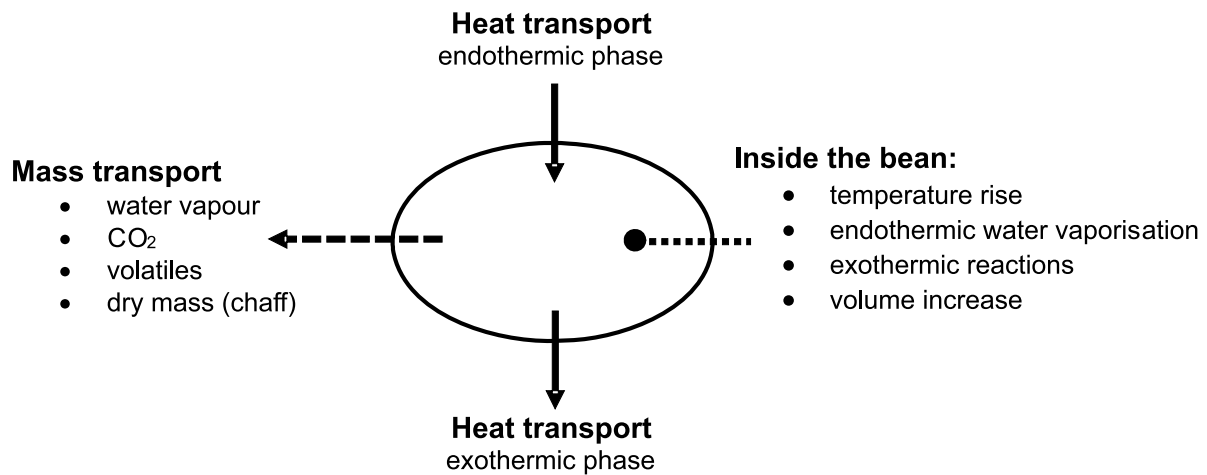


Figure 2.2: Basic coffee roasting process (adapted from Eggers & Pietsch, 2001).

2.2.1.1 Bean behaviour during roasting

At the beginning of roasting, as the coffee bean takes up more heat, a slow release of water and volatile substances occur. As this happens the internal temperature of the bean starts to rise and the chlorophyll inside the bean starts to degrade, initiating the colour change from green to yellow (Franca *et al.*, 2005; Rao, 2014).

As roasting progresses, the complexity of the roasting process is revealed when hundreds of chemical reactions start to occur simultaneously, resulting in significant changes to the bean's chemical and physical properties. Some of the more recognisable reactions include pyrolysis, Maillard reaction, Strecker degradation as well as the degradation of polysaccharides, chlorogenic acids, proteins and trigonelline (Franca *et al.*, 2005; Putranto & Chen, 2012; Sunarharum *et al.*, 2014). During the Maillard reaction, free amino acids (from the coffee bean's proteins and peptides) start to interact with the reducing sugars in the coffee bean. This forms nitrogenous heterocycles and brown melanoidins, which initiates the colour changes from yellow to tan to light brown (Flament, 2002; Rao, 2014).

During this stage, the bean experiences a rapid rise in temperature due to the occurrence of exothermic reactions. Throughout these reactions CO₂ is generated which is partially retained within the bean's cells, increasing the pressure within the bean causing the bean to expand in size (Schwartzberg, 2002; Wang & Lim, 2014). The amount of CO₂ generated is greatly dependent on the coffee type and the conditions under which it is roasted. Large amounts of CO₂, along with some water and volatile substances, are released (with an audible cracking or popping sound) as the pressure within the bean becomes too high and the bean doubles in size while it becomes half as dense, due to the formation of internal pores and pockets as the gases are released (Anderson *et al.*, 2003; Schwartzberg, 2002). It is thought that the structural changes that occur during roasting, which includes the decrease in weight and

density, increase of bean size and the expansion of internal pores, is directly connected to the amount of CO₂ generated and released (Anderson *et al.*, 2003).

All these reactions that take place inside the coffee bean during roasting, produces large amounts of volatiles, and more than 800 different compounds can develop in roasted coffee; all of these attributing to the final aroma and flavour of the coffee bean (Franca *et al.*, 2005; Schenker *et al.*, 2002). During these reactions the caramelisation of the sugar inside the coffee bean takes place, turning the coffee from the light brown to a darker brown (Rao, 2014).

As the roasting process continues and the bean temperature increases, most of the compounds within the bean has been degraded and the cell structure within dries out and weakens further. After the initial release of CO₂, the pressure inside the bean begins to build again due to the still ongoing reaction and formation of gases. A second crack, again characterised by a cracking sound, is reached when the pressure again becomes too high and along with the release of gases, internal oils are forced to the surface of the beans. The second crack further weakens the cell structure making the coffee bean brittle and light in weight (Hoffmann, 2014; Moldvaer, 2014).

2.2.1.2 Parameters influencing the roasting process

The coffee roasting process is influenced by many different factors. For instance, if not enough heat is transferred at the beginning of the roasting process (which may be due to the roaster type used or the conditions of the roasting air) the coffee beans will not dry sufficiently allowing for uneven roasting to occur during later stages and the optimal coffee flavour will not be reached (Hoffmann, 2014; Rao, 2014). Another factor that can influence roasting is the composition of the green coffee bean, which is highly dependent on the climate it is grown in and which has great influence over the internal structure of the beans, the processing method used as well as the bean's species and origin (Belitz *et al.*, 2009; Sunarharum *et al.*, 2014). Figure 2.3 illustrates the various factors that can influence the coffee roasting process.

2.2.2 Roasting technology

Modern coffee roasters work on the basis of hot roasting gas passed through constantly mixed beds of coffee beans or through streams of beans cascading or suspended in the roasting air. In most roasters, the roasting air is heated by an open flame and the main source of heat transfer is convection from the hot air to the beans (Eggers & Pietsch, 2001; Schwartzberg, 2002). During roasting, the silverskin will flake off the coffee beans (known as chaff) and be carried away by the hot air, therefore the hot air leaving the roasting chamber is usually passed through a cyclone where the chaff is separated from the air. After the separation the air is either discharged into the atmosphere, directed back to the open flame for reheating or sent through an afterburner to oxidise any volatile compounds or CO in the roasting air

(Schwartzberg, 2002, 2013). Various roasting methods exist, however the two most frequently used methods include roasting in a rotating drum and roasting in a fluidised bed (Hoffmann, 2014).

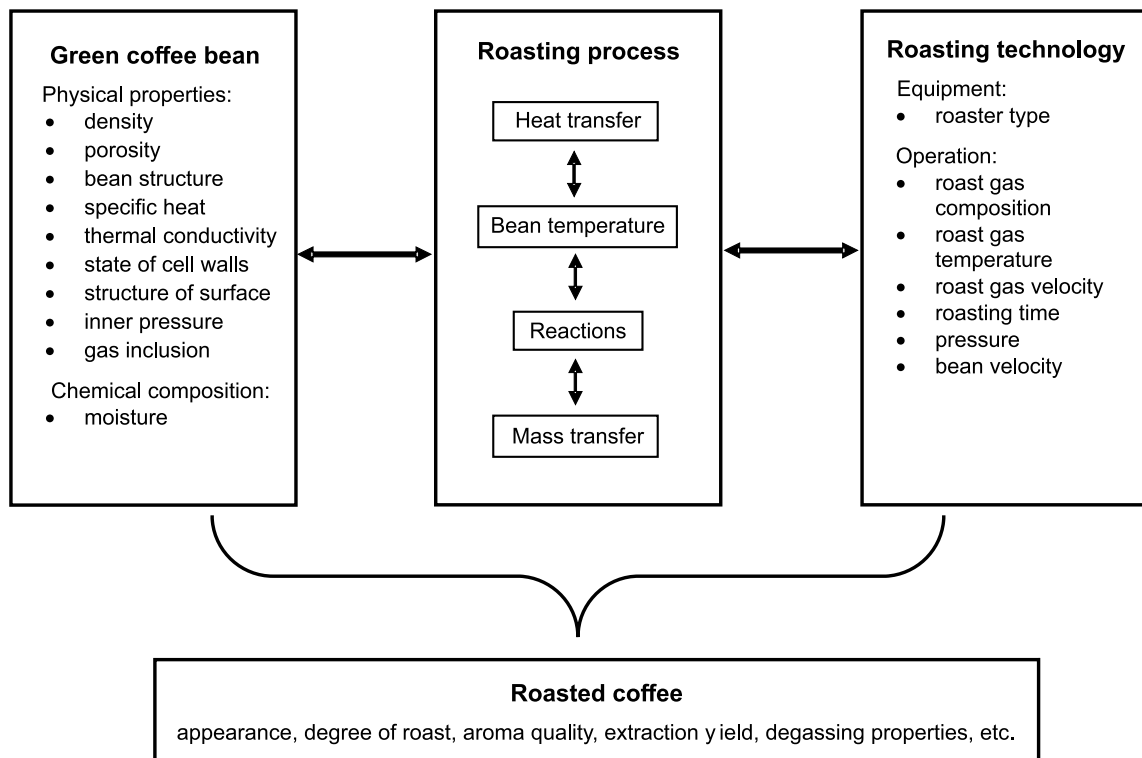


Figure 2.3: Factors influencing the roasting process (adapted from Eggers & Pietsch, 2001).

2.2.2.1 Rotating drum roasters

The rotating drum roaster is one of the most commonly used roasters today, especially by craft roasters, for it enables them to roast at slower speeds. It consists of a horizontal roasting drum with spiral flights running along the inside of the drum in order to axially mix the beans (Hoffmann, 2014; Schwartzberg, 2002). Inside the roasting chamber (rotating drum) heat is transferred by conduction, as the beans come into direct contact with hot metal surfaces, and convection, as the hot air flows through the drum. As the drum rotates above an open flame, it allows the coffee beans to continuously move during the process, effectively aiding in a more even roast (Hoffmann, 2014; Rao, 2014).

A disadvantage of the rotating drum roaster is the high temperatures needed for long roasting times (known as the high temperature/long time or HTLT roasting) to roast the beans effectively. Roasting in a drum roaster can take up to 18 minutes which can cause some beans to scorch, and often leaves oil and char deposits on the chamber walls. Due to the nature of the roaster, this is difficult to clean causing later roasts to develop a pungent, smoky taste (Eggers & Pietsch, 2001; Nagaraju *et al.*, 1997; Putranto & Chen, 2012).

2.2.2.2 Rotating bowl roasters

In a rotating bowl roaster, the coffee beans are fed into the middle of the bowl where it is driven to the edge by centrifugal forces and the hot roasting air. As the beans reach the top of the bowl, it collides with the fixed cover falling back to the centre of the bowl (Clarke, 1987; Schwartzberg, 2002). Rotating bowl roasters utilises very short roasting times, and a roast can be completed within 2 minutes. At these high roasting speeds less weight loss occurs, increasing the weight of the roasted beans that can be used. Unfortunately, high-speed roasting does not produce the best possible roasted coffee (Hoffmann, 2014).

2.2.2.3 Fluidised bed roasters

The heat transfer that takes place in a fluidised bed roaster is almost exclusively by convection. High volumes of air, preheated by and open flame, enters the roasting chamber at the bottom, where the hot air simultaneously circulate and heat the moving beans. The high volumes of air are needed to keep the beans airborne (Eggers & Pietsch, 2001; Rao, 2014). The roasting process is significantly shorter in a fluidised bed roaster than a drum roaster, due to the higher volume of air that passes through the roasting chamber, making the fluidised bed roaster a high temperature/short time (HTST) roasting process. Fluidised bed roasters have a lower risk of bean-surface burning, due to minimum or no contact with hot metal surfaces inside the roaster, producing a more uniform roasted batch of beans (Hoffmann, 2014; Nagaraju *et al.*, 1997; Rao, 2014).

A variant of the fluidised bed roaster is the spouted bed roaster, where all the beans are not fluidised equally but spouts of high-velocity air carry the beans to the top of the roasting drum where after it drops back to the bean bed. These roasters require less hot air, but the spouting actually increases the heat transfer that takes place. This method, however, tends to produce an inhomogeneous roasted batch of coffee beans (Eggers & Pietsch, 2001; Nagaraju *et al.*, 1997).

2.2.3 Stages of the coffee roasting process

In general, there are five stages that take place during roasting. These stages are termed the drying, yellowing, first crack, roast development and second crack stages, as discussed in detail below. Figure 2.4 illustrates the bean colour development as a consequence of the different roasting stages.

The speed at which these stages are reached during roasting is defined as the roast profile (as detailed in Section 2.2.4). This roast profile needs to be carefully tracked so that each roast can be reproduced within the limits of time and temperature (Hoffmann, 2014).

These roasting stages are an oversimplification of the roasting process for the purpose of making a very complex process more understandable and manageable. Therefore it should be mentioned as an example that moisture loss does not begin and end during the drying stage, but occurs continuously throughout the entire roasting process. It is just the primary change that occurs during that stage and is true for all other changes that can occur during roasting (Rao, 2014).

2.2.3.1 Stage 1: Drying

During the roasting process, coffee beans change from a light green colour to a dark brown. However this cannot happen in the presence of water and since raw coffee beans generally consist of 7 – 11% moisture evenly spread throughout the beans dense structure, the water first needs to evaporate (Hoffmann, 2014). When the roast is started a large quantity of energy and heat is required, for it takes a certain amount of time for the coffee beans to absorb enough heat for evaporation to start.



Figure 2.4: Bean colour development during the roasting process.

2.2.3.2 Stage 2: Yellowing

The coffee beans start to change in colour once enough moisture has evaporated. It is during this stage that sugars are broken down to form acids and the beans give off a bread like aroma. As this stage progresses the coffee beans will start to expand in volume, this leads to the beans' silverskin cracking off and producing chaff (Hoffmann, 2014; Rao, 2014). During the roasting process, the chaff needs to be separated from the beans to prevent the risk of fire. This is achieved by the air flowing through the roaster (Hoffmann, 2014).

The drying and yellowing stages are very important for an effective roast, for if the appropriate amount of moisture does not evaporate properly the beans will not roast evenly throughout the process. Excess moisture might allow the outside of the bean to roast properly, however the inside may stay “undercooked”. This produces a very unpleasant bitter as well as sour tasting coffee (Hoffmann, 2014). Once this happens during a roast it cannot be fixed by slowing the development of the next stages, for different parts of the bean develops at different rates (Hoffmann, 2014).

2.2.3.3 Stage 3: First crack

An accumulation of gases, which consists of mostly carbon dioxide as well as some water vapour, takes place inside the bean once the colour change progresses more rapidly. The accumulation of gases increases the pressure inside the bean until such a point where it becomes too high and the bean breaks open, commonly known as the first crack (Hoffmann, 2014). At this point, a popping sound can be heard and the bean expands to nearly double its original volume. The first crack usually happens when the roast temperature reaches 175 to 185 °C (Gloess *et al.*, 2014; Hoffmann, 2014). The popping sound starts off very slowly and quietly as the first few beans crack open and as more beans reach this point the noise will accelerate until it reaches a point from where it will begin to taper off. It can take up to 2 minutes for the first crack to begin and end, however, the higher the temperature at which roasting takes place, the shorter the first crack will be (Rao, 2014; Wang & Lim, 2012).

After the first crack is heard the roast can be stopped at any time, for it is at this stage that the coffee flavours develop. Despite still adding the same amount of heat to the roaster, the rate at which the coffee beans’ temperature increase will have a noticeable decrease at this point. However, if not enough heat is added, the coffee beans will stop to roast and instead begin to bake, which will result in a poor quality roast (Gloess *et al.*, 2014; Hoffmann, 2014).

2.2.3.4 Stage 4: Roast development

Once the first crack is reached the distinctive aroma attributed to coffee has developed. This development stage determines the roast degree and therefore bean colour of the end roast. The artisanal roaster is now in control of the balance between acidity and bitterness in the final product, for as the development continues the acid inside the beans are rapidly degrading as the bitterness of the bean start to increase (Hoffmann, 2014).

2.2.3.5 Stage 5: Second crack

Once again the beans will start to crack due to continued CO₂ build-up, however this time it is a softer snappier sound and usually happens when the roast temperature reaches values above 200 °C (Gloess *et al.*, 2014; Hoffmann, 2014; Rao, 2014). At this stage, oils are driven

to the surface of the beans and can be seen bubbling out of the bean pores. All of the acidity has degraded and a generic roast flavour has developed as a result of charring or burning. Therefore, when the second crack is reached, the quality of the coffee is of no concern for most of the characteristics of the raw coffee beans and intrinsic flavours developed during roasting has been lost, with the end product being high in body and bitterness (Hoffmann, 2014).

2.2.4 Roasting process control and the roast profile

During commercial roasting, the artisan roaster continuously evaluates the progression of the roast. This is done by continuously examining several parameters of the process as the roast progress through the above-mentioned stages (Heyd *et al.*, 2007). The artisan roaster interprets the observable parameters (such as bean colour, sound of first and second crack, and aroma formation) throughout the roast and compares it to the measured roast profile in order to determine necessary adjustments (increasing or decreasing air flow and air temperature) that should be made to achieve a specific end product quality (or degree of roast) (Hernández *et al.*, 2007; Putranto & Chen, 2012).

Since most roasts will not exceed 20 minutes, these adjustment needs to be made almost instantaneously for the desired effect to happen. No set rules exist to produce a specific roast, and it takes years of learning and experience to be able to evaluate the roast and incorporate the correct adjustments to produce a superior quality product. Another objective in the control of the roasting process is to consistently reproduce the roast profile to obtain the same quality product when desired (Yeretzian *et al.*, 2012). Figure 2.5 illustrates a typical roast profile as it progresses through the above-mentioned stages. With most commercial coffee roasters equipped with thermocouples measuring the roast profile, the measuring of this temperature profile can quite easily be used in conjunction with a desired roast profile in a control strategy to achieve a perfect roast.

The roast profile is defined as the evolution of the bean-probe temperature as the roasting process progresses. Commercial roasters measure this temperature with a thermocouple inserted into the bean bed. This, however, is not to be confused or interpreted as the internal or surface temperatures of the bean, for it merely measures the temperature of the medium surrounding it which, in this case, is a mixture of coffee beans and hot air (Rao, 2014; Schwartzberg, 2002).

The beginning temperature of the roast profile is the temperature of the hot air the moment the beans enter the drum and the immediate drop in temperature at the beginning of the roast profile, as illustrated in Figure 2.5, is just the logical interaction of beans at room temperature coming into contact with an environment at a higher temperature (Rao, 2014)

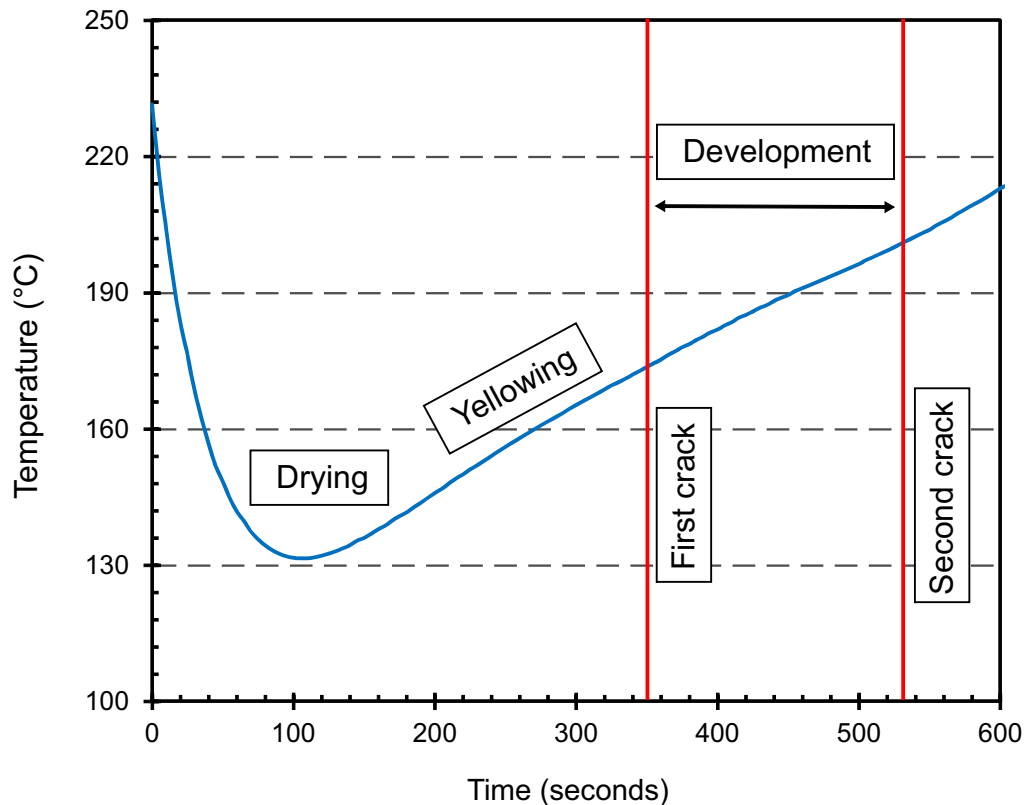


Figure 2.5: A typical roast profile in terms of the roasting stages (adapted from Rao, 2014).

2.2.5 The degree of roast

After roasting is done, the quality of the roasted coffee needs to be evaluated and classified. The degree of roast is normally based on the bean colour, though the exact roast level that each roast degree indicates is not agreed upon and can vary from roaster to roaster (Rao, 2014). Various different labels exist (as seen in Table 2.2), however for the purpose of simplification the degree of coffee roasting is categorised into the general light, medium, dark and very dark roast (Santos *et al.*, 2016; Wang & Lim, 2014). Table 2.2 gives a description of the various roast degrees in terms of the beans' progression through the roasting stages as well as their general appearance.

Over the years numerous research activities focussed on the determination of the roast degree based on various physical properties of the roasted coffee, i.e. colour development of the bean, weight loss during the roasting process (more commonly referred to as roast loss), chemical composition of roasted beans and the final moisture content of the bean (Alessandrini *et al.*, 2008; Baggenstoss *et al.*, 2008; Wang & Lim, 2014).

It is found, however, that the composition of green coffee beans is highly dependent on various factors including cultivation climate, processing method, bean species and origin and the roasted beans are further dependent on the extent of roasting (Belitz *et al.*, 2009). Therefore it is not seen as a suitable way to compare various compositions to obtain the roast degree.

Table 2.2: Classification of roast degree (adapted from Hoffmann, 2014; Rao, 2014).

Roast degree	Roast progression	Appearance	General degree
Cinnamon roast	Extracted at the very beginning of first crack	Light brown, cinnamon colour	Light roast
City roast	Extracted at the last stages of, or just after, first crack	Smoother surface due to expansion	
Full city roast	Extracted just before the start of second crack	Slight appearance of surface oils	Medium roast
Viennese roast	Extracted at the very beginning of second crack	Noticeable presence of surface oils	
French roast	Extracted during second crack	Dark brown and very oily	Dark roast
Italian roast	Extracted at the end of, or just after, second crack	Dark brown almost burnt	Very dark roast

2.2.5.1 Colour

The most commonly used measurement to determine the roast degree is the bean colour. The colour of coffee is usually measured with a photometer or colorimeter, and the measured values are expressed in the CIE $L^*a^*b^*$ space (a widely accepted international standard for colour determination implemented by the Commission Internationale d'Eclairage (CIE)). The parameters a^* (green to red) and b^* (blue to yellow) are the chromatic components (Gokmen & Senyuva, 2006). The L^* - value, which states the lightness of the colour, is used to determine the degree of roast. L^* - value of 0 signifies black colour where a value of 100 signifies white (Baggenstoss, Perren, *et al.*, 2008; Baggenstoss, Poisson, *et al.*, 2008b). Table 2.3 shows average values that have been determined for the various roast degrees.

Table 2.3: Colour values for different roast degrees (adapted from Baggenstoss, Poisson, *et al.*, 2008b; Schwartzberg, 2013).

General degree	L^*
Light roast	28-30
Medium roast	24
Dark roast	20-21
Very dark roast	18

2.2.5.2 Moisture content

The final moisture content of the coffee beans can be an indication of roast degree, for as the roasting process progresses, more and more water evaporates from within the coffee beans.

Table 2.4: Moisture content for different roast degrees (adapted from Baggenstoss, Poisson, *et al.*, 2008b; Eggers & Pietsch, 2001).

General degree	Moisture (wt%)*
Light roast	2.8
Medium roast	2.0
Dark roast	1.7
Very dark roast	1.4

*On a wet basis

2.2.5.3 Roast loss

The percentage weight loss, also called the roast loss (RL), during roasting can indicate how well the bean core is penetrated during a particular roast and can give an indication of roast development. The higher the RL percentage the more developed the roast and therefore the darker the degree of roast (Rao, 2014). The weight loss of the coffee beans during the roasting process can, therefore, be an indication of the degree of roast, however it can only be an end result indication and not a continuous observation during roasting, for it is extremely difficult to determine weight loss on-line in commercial roaster (Hernández *et al.*, 2007). Table 2.5 gives average values of the percentage RL for varying roast degrees.

Table 2.5: Percentage roast loss for different roast degrees (adapted from Baggenstoss, Poisson, *et al.*, 2008b; Cho *et al.*, 2014; Eggers & Pietsch, 2001; Schwartzberg, 2013).

General degree	Roast loss %
Light roast	10-13
Medium roast	14-16
Dark roast	17-20
Very dark roast	<22

2.3 Roasting models

For the optimisation of the coffee roasting process, the temperature and moisture evolution in coffee beans during this process needs to be studied. In recent years, many researchers have focussed on this by investigating the heat and mass transfer during the roasting of green coffee beans and proposing a model which can predict the temperature and moisture evolution within the beans. These researchers include Basile & Kikic, (2009); Fabbri *et al.*, (2011);

Hernández-Díaz *et al.*, (2008); Heyd *et al.*, (2007); Putranto & Chen, (2012) and Schwartzberg, (2002).

Schwartzberg (2002) developed a semi-physical model to predict the bean temperature and moisture content of the coffee bean during a batch roasting process, as well as the measured temperature of the batch of beans. In later years, Hernández *et al.* (2007), Bottazzi *et al.* (2012) and Alonso-Torres *et al.* (2013), all used Schwartzberg's model to investigate its correlation with experimental data. They all found that the model was effective in predicting the bean temperature and moisture content of the beans during roasting.

Heyd *et al.* (2007) proposed a dynamic model to describe the heat and mass transfer in a spouted bed roaster. This model included the heat and mass transfer at the surface of the beans as well as inside the beans. According to the authors, this model had a good correlation between the predicted and experimental data, however this correlation could only be obtained when the water diffusivity of the bean was adjusted.

Basile & Kikic (2009) used a lumped specific heat capacity approach to develop a model to predict the non-stationary thermal profile of the coffee beans during the roasting process. In this model, the assumption was made that the thermal effects which occur in the coffee beans during roasting can be contained in a lumped together specific heat parameter.

All the models described above used a simplified geometry to define the coffee bean structure. They particularly used semi-ellipsoids and spheres. Fabbri *et al.* (2011) proposed a numerical model predicting the heat and mass transfer during the coffee roasting process based on a three-dimensional geometry.

Putranto & Chen (2012) used the lumped-reaction engineering approach to develop a coffee roasting model, from which details of the process kinetics could be captured. This approach assisted in a more realistic assessment of the moisture loss, for it evaluated the average moisture content instead of assuming a uniform moisture content.

In the following section the heat and mass transfer models proposed by Fabbri *et al.*, (2011); Heyd *et al.*, (2007); Putranto & Chen, (2012) and Schwartzberg, (2002) will be discussed along with any results that were obtained to validate the predictive capability of the models.

2.3.1 Schwartzberg (2002) model

Schwartzberg (2002) proposed a model based on Equation 2.1, which modelled the average temperature of the beans (T_b) during the roasting process. Equation 2.1 included the heat transfer from the hot roasting gas to the beans (Q_{gb}), as well as heat lost due to heat transfer from the hot gas to the metal of the roaster (Q_{gm}). Since most industrial roasters have some parts where there are bean on metal contact, the equation also included heat transfer from

hot metal parts to the beans (Q_{mb}) (Schwartzberg, 2002). However, the use of the latter two terms are greatly influenced by the type of roaster used during the roasting process and in most cases they can be neglected due to the nature of the heat transfer.

$$\frac{dT_b}{dt} = \frac{Q_{gb} - Q_{gm} + Q_{mb} + m_b \left(Q_r + \Delta H_v \frac{dX_b}{dt} \right)}{m_b(1 + X_b)Cp_b} \quad \text{Equation 2.1}$$

Research conducted by Raemy (1981) and Raemy & Lambelet (1982) found that during the heating of coffee beans (using differential thermal analyses) some exothermic reactions will take place and that a significant amount of heat is generated by these reactions. Therefore Equation 2.1 also accounted for the heat generated by exothermic roasting reactions (Q_r) (Schwartzberg, 2002).

The heat generated by exothermic reactions are calculated using Equation 2.2, however little to no explanation is given with regards to the values used in this equation and Schwartzberg (2002) made use of constant values, stating their use during later modelling calculations.

$$Q_r = Ar \cdot \exp \left[\frac{Ha}{R(T_b + 273.2)} \right] \left(\frac{H_{et} - H_e}{H_{et}} \right) \quad \text{Equation 2.2}$$

From this, it is concluded that these values were in fact estimated during modelling to ensure the best fit to the experimental data and that no experimental means was used to corroborate these values.

Another important aspect when modelling the roasting process is the moisture loss during roasting. Schwartzberg (2002) proposed Equation 2.3, a semi-empirical equation, to model the moisture content of the coffee beans (X_b) during roasting. This model only accounts for the evaporation of the initial moisture content of the bean and does not take into consideration water formation that may occur during the roasting reactions. With the implementation of Equation 2.3 it was assumed that the moisture loss was diffusively controlled and that an Arrhenius type equation governed the temperature dependency of the diffusion coefficient (Bottazzi *et al.*, 2012; Schwartzberg, 2002).

$$-\frac{dX_b}{dt} = \frac{4.32 \times 10^9 \cdot X_b^2}{d_b^2} \exp \left[\frac{-9889}{T_b + 273.2} \right] \quad \text{Equation 2.3}$$

This equation is based on corrected moisture loss data which were obtained from experimental roasting data that were adjusted to exclude any moisture increase due to reaction based water formation (this was done by subtracting any estimated increase in moisture from the obtained data).

A commercial coffee roaster measures the temperature of the bean batch using a thermocouple inserted into the coffee bed. This is most commonly referred to as the roast profile. As coffee beans are poor conductors of heat, there exist an obvious difference between the bean temperature (which is modelled by Equation 2.1) and the measured bean batch temperature, or roast profile (Rao, 2014; Schwartzberg, 2002). Therefore Schwartzberg (2002) suggested Equation 2.4 to model the roast profile (T_{rp}) during the roasting process.

$$\frac{dT_{rp}}{dt} = K(T_b - T_{rp}) \quad \text{Equation 2.4}$$

Schwartzberg (2002) used Equation 2.1 to Equation 2.4 to simulate the bean temperature as well as the roast profile for the roasting of 400 kg of green coffee beans in a rotating-bowl roaster. The results obtained from the model were compared to those obtained from an experimental roast, where the roast temperature was recorded at ten second intervals. These results are shown in Figure 2.6.

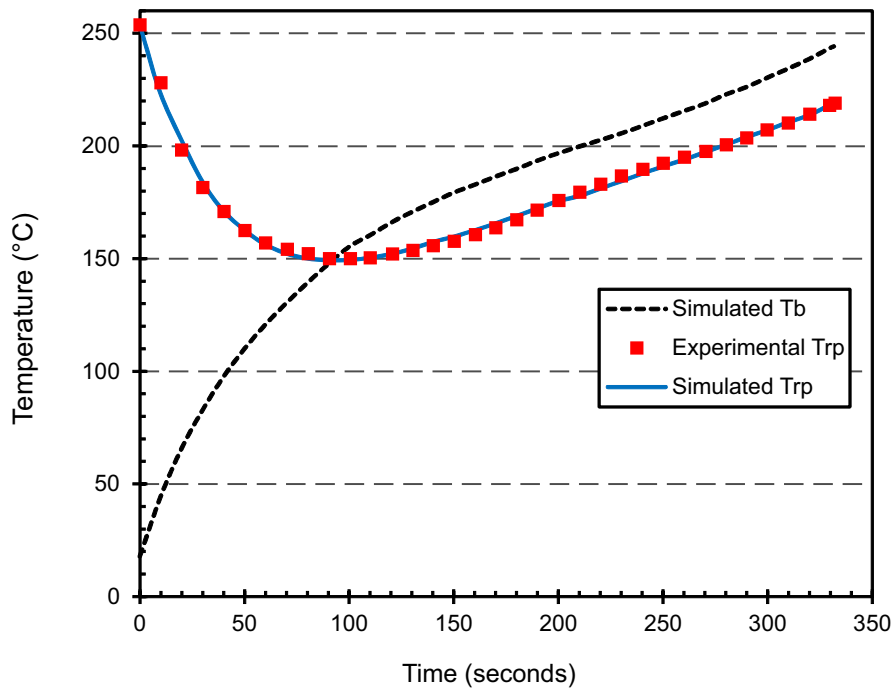


Figure 2.6: Simulated results compared to experimental results obtained by Schwartzberg (2002).

Schwartzberg (2002) found that the simulated roast profile was in a good agreement with that of the experimental roast profile during the entire process, and that the largest difference in temperature between the simulated and experimental data was only 2 °C, as depicted in Figure 2.6. Schwartzberg (2002) did not include any results obtained regarding the moisture loss of the green coffee beans during the roasting process, therefore the proposed equation for moisture loss could not be verified from his work. However in later years Hernández *et al.*

(2007), Bottazzi *et al.* (2012) and Alonso-Torres *et al.* (2013), all used Schwartzberg's model to investigate its correlation with experimental data.

Hernández *et al.* (2007) did roasting experiments where the bean temperature was measured with thermocouples inserted into green coffee beans, however, no specific roaster was used and 25 grams of green beans were just introduced into hot air for roasting. The roasting setup was constructed in such a way that the beans' weight was automatically measured in one minute intervals during the roasting process. Hernández *et al.* (2007) found that the simulated results from the model had an overall good fit compared to experimental results, however, compared to the experimental results the moisture loss model significantly underestimated the coffee beans water content after 300 seconds. According to Hernández *et al.* (2007), this may be due to the fact that the model only considers moisture loss as the total weight loss and not the true weight loss consisting of volatile, water and CO₂ release. Hernández *et al.* (2007) on the other hand did not determine the moisture content of the coffee beans and instead used the weight loss results obtained at one minute intervals as a comparison with the simulated moisture content. Considering that weight loss included moisture and gas release, the obtained experimental results should give significantly lower results than those of the simulated moisture loss model.

Both Bottazzi *et al.* (2012) and Alonso-Torres *et al.* (2013), used the model proposed by Schwartzberg (2002) to simulate the roasting process and compare its results with experimental results obtained by Schenker (2000). The roasting experiments were conducted in a fluidised bed laboratory roaster in 100 grams green coffee bean batches. The bean temperature was determined by thermocouples inserted into the green coffee beans, which were in fixed positions inside the roaster. To analyse the moisture content during the roasting process, samples were extracted at regular intervals (Schenker, 2000).

Alonso-Torres *et al.* (2013) found that the moisture loss simulated with the model compared fairly well with the experimental moisture loss results, however throughout the entire process the simulated data had a slightly higher estimated value.

Bottazzi *et al.* (2012) used the model to simulate bean temperature and moisture content for a roasting process with air temperatures ranging from 220 to 260 °C (because of the higher air temperature of 260 °C the roasting process will progress faster than at lower air temperatures), and found that the simulated bean temperature compared fairly well with that of the experimental bean temperature, as illustrated in Figure 2.7.

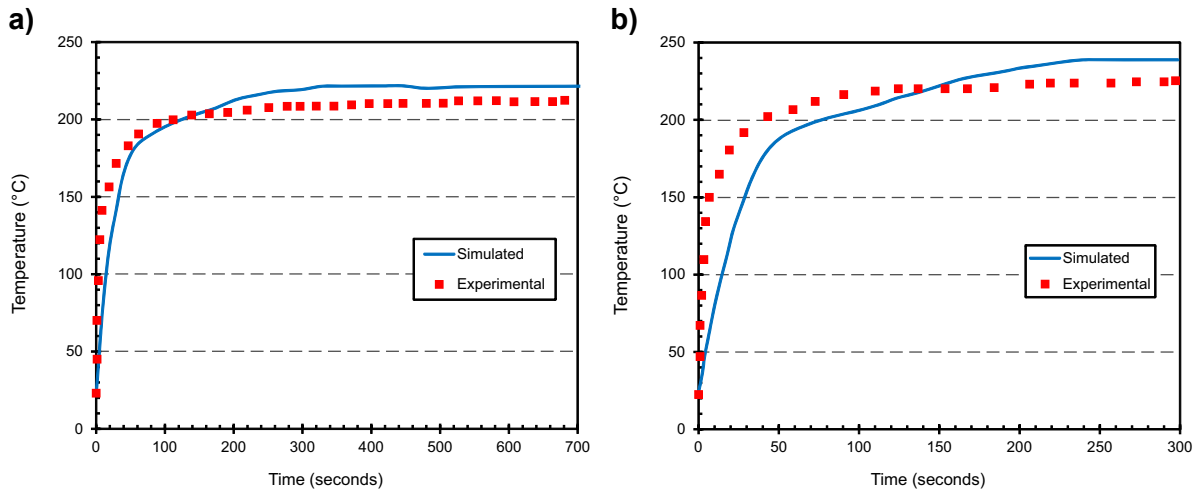


Figure 2.7: Simulated bean temperature compared to experimental results for a) air temperature of 220 °C and b) air temperature of 260 °C (taken from Bottazzi *et al.*, 2012).

The simulated moisture content of coffee beans was in a good agreement with the experimental results and is shown in Figure 2.8. Although at higher temperatures the model did overestimate the initial time needed for the evaporation of the moisture from the beans to start. It was concluded that the proposed moisture loss model was more accurate with a longer roasting cycle compared to that of a faster one (Bottazzi *et al.*, 2012).

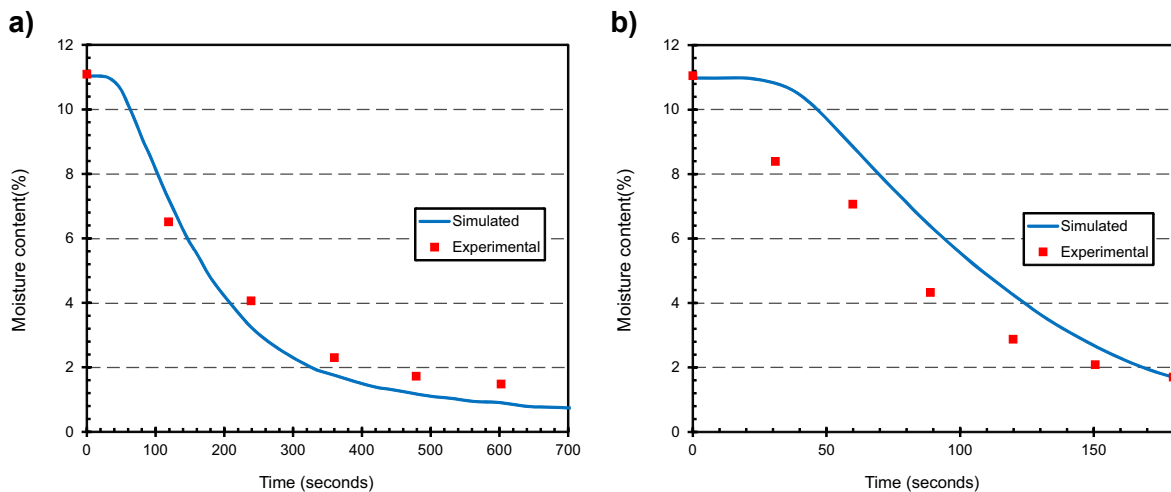


Figure 2.8: Simulated moisture content compared to experimental results for a) air temperature of 220 °C and b) air temperature of 260 °C (taken from Bottazzi *et al.*, 2012).

2.3.2 Heyd *et al.* (2007) model

Heyd *et al.* (2007) aimed to develop a more accurate model (than that of Schwartzberg (2002)) that could better describe the roasting process, and consequently determine the bean temperature and bean moisture more accurately during roasting. To ensure that the proposed model can be implemented during predictive control of the roasting process, the accuracy of the predicted bean temperature is of great importance. For that reason, an output gas temperature (which can easily be measured in a commercial roaster) prediction is also

included in the proposed model. The comparison between the measured and simulated output air temperature can help with on-line validation of simulated bean temperature during roasting (Heyd *et al.*, 2007).

Assuming that the water diffusivity is uniform in space and that it stays constant during the entire roasting process, the moisture loss model is given by Equation 2.5, where a spherical geometry is taken into account. Equation 2.5 also neglects any water formation due to roasting reactions (Heyd *et al.*, 2007). This equation is used in conjunction with boundary conditions to simulate the moisture content of coffee beans during the roasting process.

$$\frac{\partial X_b(r, t)}{\partial t} = D \left[\frac{\partial^2 X_b}{\partial r^2} + \frac{2}{r} \frac{\partial X_b}{\partial r} \right] \quad \text{Equation 2.5}$$

Heyd *et al.* (2007) proposed Equation 2.6, which describes heat conduction within a sphere, to model the bean temperature. This equation is based on the assumptions that the exothermic roasting reactions do not produce any heat and that the effect of heat transported by water within the bean can be neglected. Specifying the boundary conditions for Equation 2.6 will allow for the bean temperature to be simulated with this model.

$$\rho_b(Cp_b + X_b Cp_w) \frac{\partial T_b(r, t)}{\partial t} = \lambda_b \left[\frac{\partial^2 T_b}{\partial r^2} + \frac{2}{r} \frac{\partial T_b}{\partial r} \right] \quad \text{Equation 2.6}$$

To simulate the exhaust gas temperature, an air heat balance is considered, which accounts for the heat transported by the hot roasting air, the heat transfer that takes place between the hot roasting air and its environment (heat loss through the system), as well as the heat transferred to the coffee beans due to condensation and convection. The proposed model to simulate the exhaust gas temperature is given by Equation 2.7 (Heyd *et al.*, 2007).

$$\begin{aligned} \frac{\partial T_g}{\partial t} \rho_g Cp_g (1 - \varepsilon) \pi R_t^2 &= h_{bg} L_{bg} (T_b - T_g) + k L_{bg} (p_s - p_g) \Delta H_v \\ &+ 2\pi R_t h_{tg} (T_t - T_g) - G Cp_g \frac{\partial T_g}{\partial z} \end{aligned} \quad \text{Equation 2.7}$$

Heyd *et al.* (2007) discretized the proposed equations to obtain a system of ordinary differential equations that can be solved simultaneously. The water diffusivity coefficient used in the moisture loss model (Equation 2.5) was adapted to fit moisture content and output air temperature obtained from a roast experiment at an input air temperature of 230 °C. Roasting experiments were conducted with 100 grams of green coffee beans, roasted in a spouted bed coffee roaster. The bean temperature was measured during the roast, at one minute intervals, with a thermocouple inserted into one of the beans. Coffee beans were sampled for moisture content measurements at regular intervals. The simulated results were compared to the

results obtained from roasts conducted at input air temperatures of 210 °C and 250 °C (Heyd *et al.*, 2007).

Figure 2.9 shows that the simulated bean temperature behaves in a similar manner than the experimental temperature for both input air conditions. For the input air at 250 °C, depicted in Figure 2.9 (b), the experimental data had a slight deviation from the simulated data between 240 and 300 seconds during the roasting process. According to Heyd *et al.* (2007), this deviation from simulated results may be due to the occurrence of exothermic reactions during roasting, which was not accounted for in the proposed model.

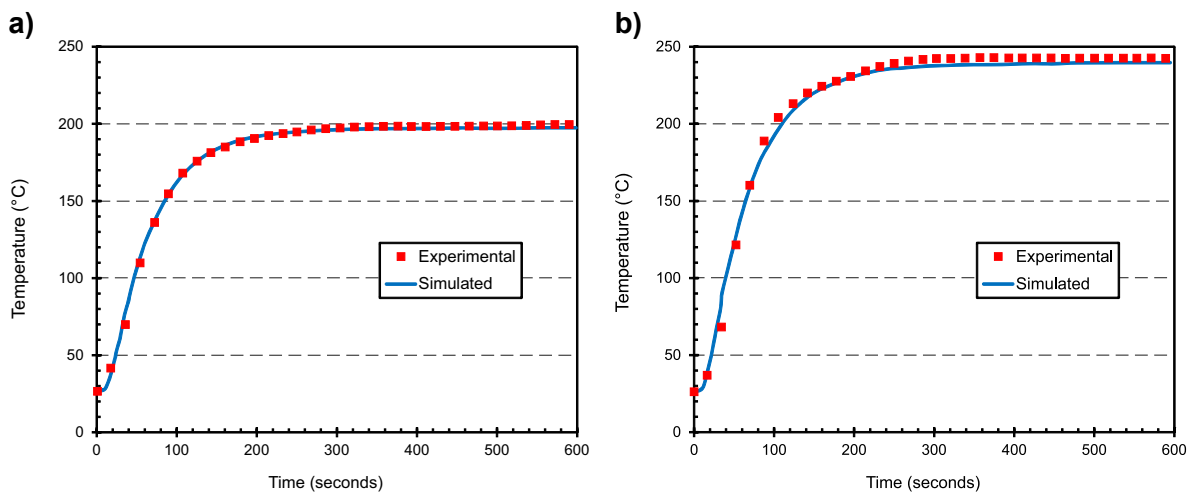


Figure 2.9: Simulated bean temperature compared to experimental results for a) input air temperature of 210 °C and b) input air temperature of 250 °C (taken from Heyd *et al.*, 2007).

The comparison between the simulated and experimental output air temperatures (for roasting at the specified air conditions) is shown in Figure 2.10. For the roasting at 210 °C, Figure 2.10 (a), a slight difference (more or less 5 °C) between the simulated and experimental temperatures can be observed during the middle of the roasting process. This deviation is corrected closer to the end of the roasting process when a more steady-state temperature is reached (Heyd *et al.*, 2007).

At the end of roasting at 250 °C, Figure 2.10 (b), the experimental output air temperature reaches about 4 °C higher than the simulated temperature. This deviation may be due to several factors, however it can be maintained that the overall simulated output air temperature compared adequately with the experimental temperatures (Heyd *et al.*, 2007).

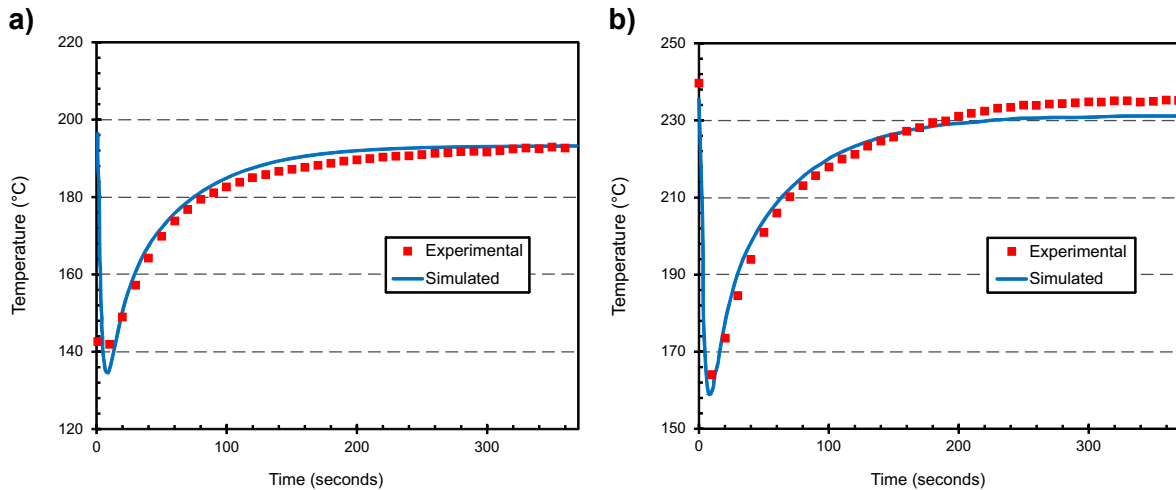


Figure 2.10: Simulated output air temperature compared to experimental results for a) input air temperature of 210 °C and b) input air temperature of 250 °C (taken from Heyd *et al.*, 2007).

Finally, the simulated moisture content was compared to the experimentally obtained moisture content, which is shown in Figure 2.11. Although the moisture loss model did not include all physical occurrences that can take place during the roasting process, such as the effect temperature can have on the water diffusivity of the bean or the water formation that can occur during roasting reactions, Heyd *et al.* (2007) found that the simulated results were in a good agreement with the experimental moisture content measured from three separate extracted samples during the roasting process.

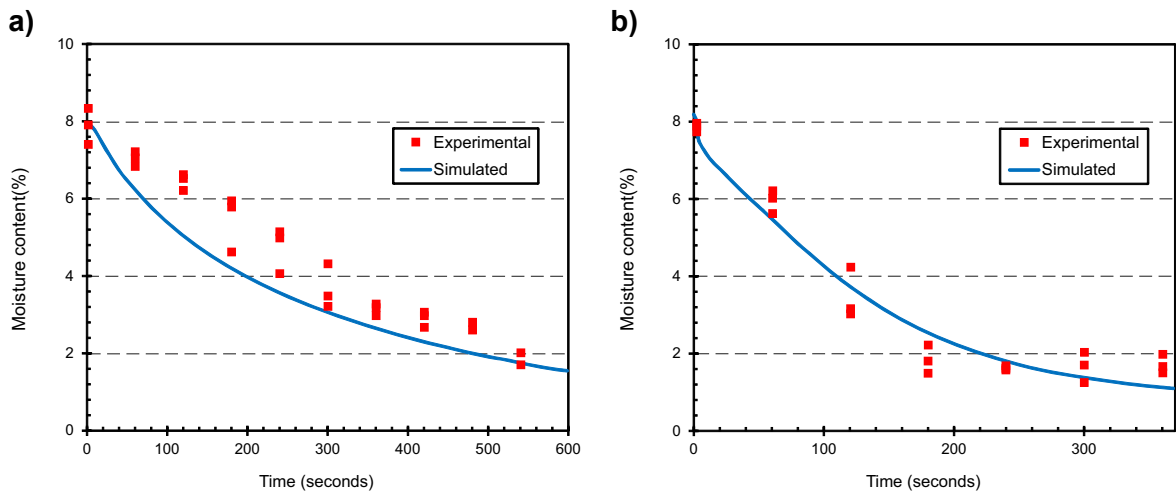


Figure 2.11: Simulated moisture content compared to experimental results for a) input air temperature of 210 °C and b) input air temperature of 250 °C (taken from Heyd *et al.*, 2007).

According to Heyd *et al.* (2007) this proposed model, with the adjusted water diffusivity coefficient, can be applied to different coffee roasters and could be a practical solution for on-line predictive control of the coffee roasting process, or even other roasting processes.

2.3.3 Fabbri *et al.* (2011) model

Fabbri *et al.* (2011) aimed to develop a numerical model, capable of simulating the heat and moisture transfer that takes place inside a coffee bean during the roasting process based on a three-dimensional digitised geometry. The digitised geometry used by the proposed model was constructed by means of a three-dimensional scan of a green coffee bean.

To model the bean temperature, Fabbri *et al.* (2011) assumed that the heat transfer that takes place during roasting is predominantly convection, from hot roasting air to the surface of the coffee bean, and conduction, that occurs from the surface of the bean towards its core. Equation 2.8 is proposed to model the heat transfer by conduction that takes place inside the bean, while a boundary condition is offered to represent the convection that occurs between the roasting air and the surface of the bean (Fabbri *et al.*, 2011).

$$\rho_b c p_b \frac{\partial T_b}{\partial t} + \nabla \cdot (-\lambda_b \nabla T_b) = 0 \quad \text{Equation 2.8}$$

The proposed heat transfer model neglects any heat that may be produced during roasting by exothermic roasting reactions, and only accounts for heat transferred from the hot roasting air (Fabbri *et al.*, 2011). Fabbri *et al.* (2011) assumed that the moisture inside the coffee bean will diffuse toward the surface and that only at the surface of the bean, the moisture will start to evaporate, while the mass transfer that takes place during roasting was assumed to be governed by Fick's law. The proposed moisture loss model, in terms of the moisture concentration inside the bean, is given by Equation 2.9.

$$\frac{\partial c_b}{\partial t} + \nabla \cdot (-D_b \nabla c_b) = 0 \quad \text{Equation 2.9}$$

According to Fick's law of diffusion, the mass flux of the diffusant is directly proportional to the gradient of concentration and the proportionality constant is the diffusion coefficient (Crank, 1975). Therefore the diffusion coefficient used is of great importance for the accuracy of the proposed model.

Hernández-Díaz *et al.* (2008) found that the water diffusivity of the coffee bean is influenced by the bean temperature and proposed Equation 2.10 to calculate the diffusion coefficient. This equation is based on experimental data fitted to an Arrhenius type equation and is used by Fabbri *et al.* (2011) in the proposed moisture loss model.

$$D_b = \exp \left(2.7085 - \frac{66856.4}{RT} + 1.74 \frac{c_{b,avg}}{c_{b,i}} \right) \quad \text{Equation 2.10}$$

To validate the proposed model, Fabbri *et al.* (2011) used a rotating drum prototype to roast green coffee beans at an air temperature of 200 °C. For the bean temperature experiments, a single green coffee bean was placed in the middle of the roaster and the temperature was measured by a thermocouple inserted into the bean. The moisture content was obtained from roasts, conducted at different time intervals to simulate different roasting stages, of 3 grams of coffee beans (Fabbri *et al.*, 2011).

Fabbri *et al.* (2011) found that the simulated and experimental bean temperature (which was obtained from five replicate roasts) compared very well with one another with a root mean square error (RMSE) of 5.97 °C. The comparison between the simulated and experimental results are shown in Figure 2.12.

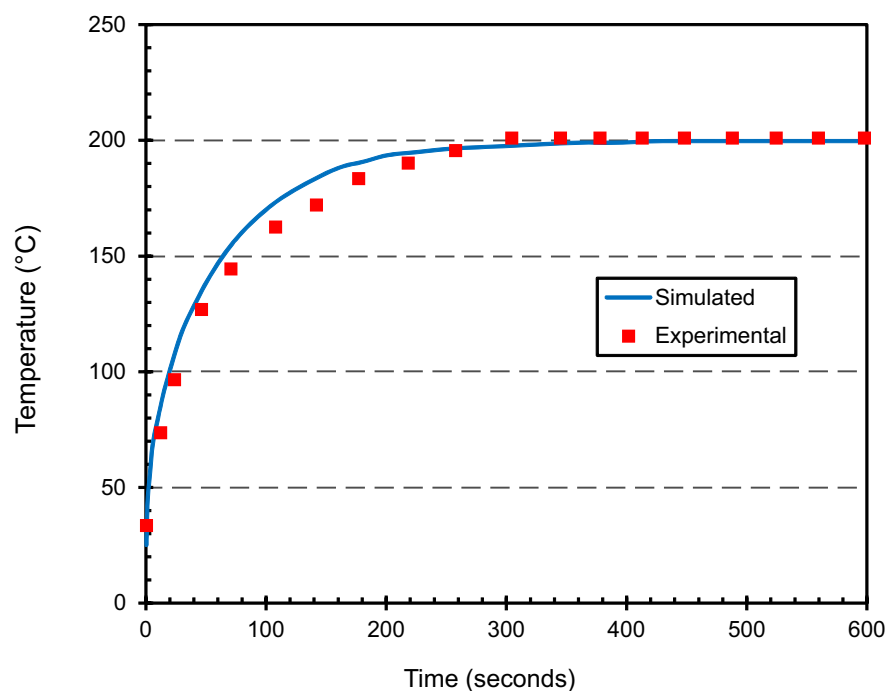


Figure 2.12: Simulated bean temperature compared to experimental results for roasting at 200 °C (taken from Fabbri *et al.*, 2011).

In Figure 2.13 the simulated moisture content compared to the experimental results for roasting at 200 °C is shown. A RMSE of 0.75 % d.b. moisture content was obtained from the compared results, showing that they appear to be in good agreement. According to Fabbri *et al.* (2011), the slight deviation between simulated and experimental results that can be observed at certain points may be due to steam produced inside the coffee bean when the bean temperature increases. In spite of these deviations, Fabbri *et al.* (2011) maintained that the proposed model predicted the moisture content of coffee beans during roasting more accurately than those proposed by Schwartzberg (2002) and Heyd *et al.* (2007).

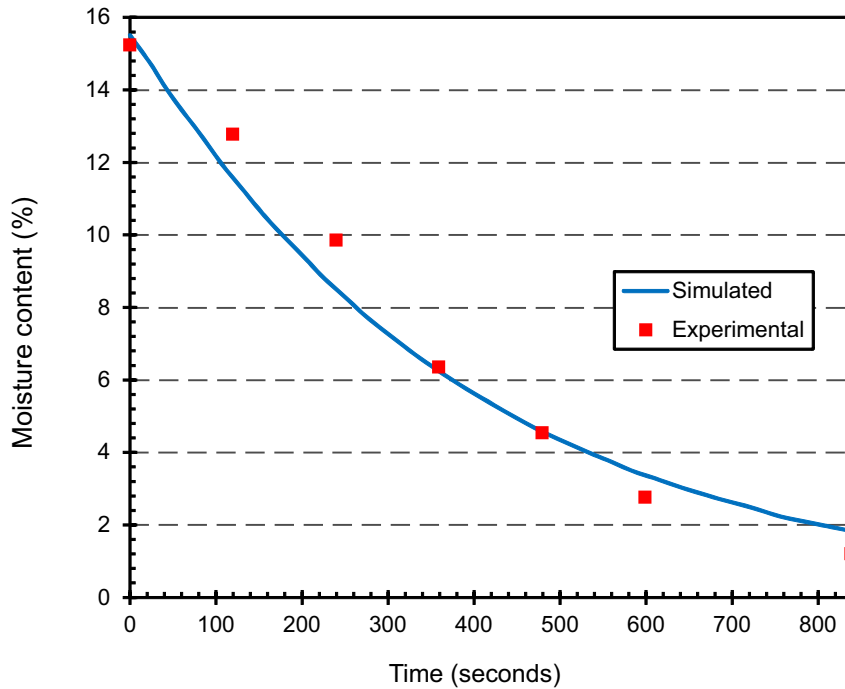


Figure 2.13: Simulated moisture content compared to experimental results for roasting at 200 °C (taken from Fabbri *et al.*, 2011).

2.3.4 Putranto & Chen (2012)

Most models proposed for the roasting process implements a diffusion-based approach, which is experimental by nature, since the diffusion coefficient needs to be determined by means of several experiments, making it moisture content and temperature dependent. According to Putranto & Chen (2012), the model proposed to simulate the roasting process needs to be robust, straightforward and accurate, and should require the least possible number of parameters determined by experiments. This would make the model more sufficient for use in the optimisation and control of the roasting process. Chen & Xie (1997) proposed one such model; the reaction engineering approach (REA).

The REA is a way to model drying kinetics by using the principles of chemical reaction engineering. This approach estimates the average moisture content instead of assuming a uniform moisture content. There are two different types of REA's, the lumped reaction engineering approach (L-REA) and the spatial reaction engineering approach (Putranto *et al.*, 2011; Putranto & Chen, 2012). Putranto & Chen (2012) proposed a heat and mass transfer model which uses the L-REA to estimate the moisture loss during the roasting process.

Putranto & Chen (2012) proposed Equation 2.11 to simulate the moisture content of the coffee beans. The L-REA is thusly named because the mass balance used for modelling the moisture loss is expressed by a lumped ordinary differential equation, as can be seen in Equation 2.11 (Putranto *et al.*, 2011).

$$\frac{dX_b}{dt} = -kA_b \left[\exp\left(\frac{-\Delta E}{RT_b}\right) p_{sat} - p_g \right] \frac{1}{m_b} \quad \text{Equation 2.11}$$

Equation 2.11 incorporates the activation energy, which signifies the added effort to remove moisture from the coffee bean, and is, in fact, dependent on the moisture content. This parameter is determined experimentally from one accurate moisture content curve obtained from a roast and is calculated using Equation 2.12 (Putranto & Chen, 2012).

$$\Delta E = -RT \ln \left[\frac{-m_b \frac{dX_b}{dt} \frac{1}{kA_b} + p_g}{p_{sat}} \right] \quad \text{Equation 2.12}$$

To simulate the moisture content and bean temperature during roasting, the proposed L-REA model is combined with a heat balance shown by Equation 2.13 (Putranto & Chen, 2012). The proposed bean temperature model is fairly similar to the one proposed by Schwartzberg (2002) (refer to Equation 2.1), however it does not take into account the heat transfer from the metal parts to the bean or the heat generated by exothermic roasting reactions.

$$\frac{dT_b}{dt} = \frac{hA_b(T_{g,i} - T_b) + m_b \frac{dX_b}{dt} \Delta H_v}{m_b(1 + X_b)Cp_b} \quad \text{Equation 2.13}$$

Putranto & Chen (2012) compared the simulated results obtained from the proposed model with the simulated and experimental results obtained by Fabbri *et al.* (2011). This was done to investigate, not just the accuracy of the proposed model compared to experimental results, but its suitability to be used instead of the one proposed by Fabbri *et al.* (2011). The simulated results compared to the results obtained from Fabbri *et al.* (2011) for bean temperature and moisture content, is shown in Figure 2.14 and Figure 2.15 respectively.

Putranto & Chen (2012) found that the simulated results of the bean temperature fit fairly well with the experimental data, which is supported by a RMSE of 4.8 °C. The slight overestimation of bean temperature by the proposed model of Fabbri *et al.* (2011) between the times of 50 and 200 seconds, was also shown by the simulated data of Putranto & Chen (2012).

The simulated moisture content had a good fit with the experimental data (supported by a RMSE value of 0.2 % d.b.), as can be seen in Figure 2.15. The proposed moisture loss model of Fabbri *et al.* (2011), underestimated the moisture content during roasting between 100 and 300 seconds. This is not observed by the L-REA model, indicating that the L-REA model gives a more accurate prediction than the diffusion based model of Fabbri *et al.* (2011) (Putranto & Chen, 2012).

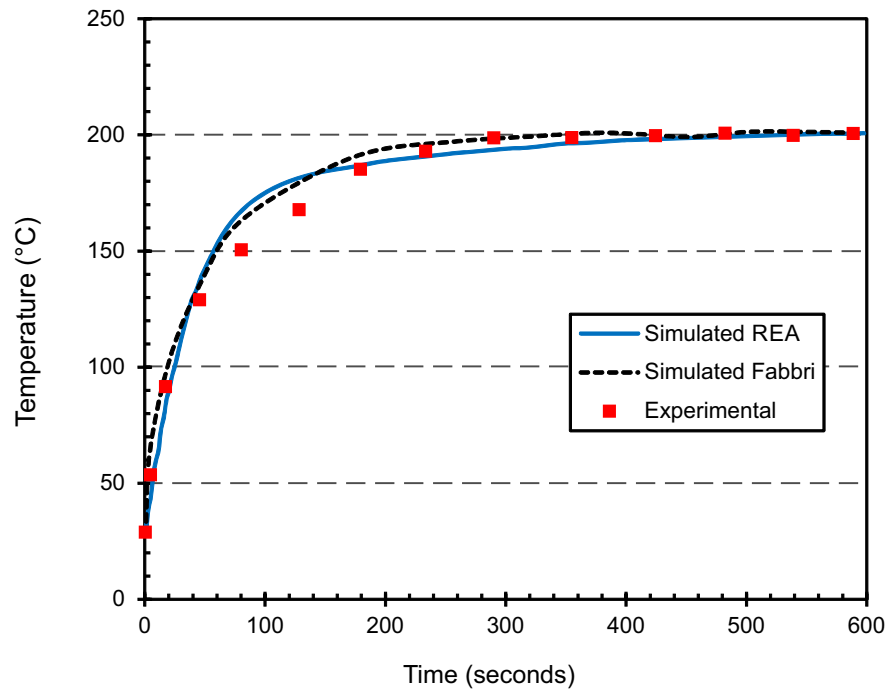


Figure 2.14: Simulated bean temperature determined by Putranto & Chen (2012) compared to results obtained by Fabbri *et al.* (2011).

Putranto & Chen (2012) found that the L-REA model is an accurate and simple way to model the coffee roasting process. With its small number of experimentally determined parameters, accurate results and minimum amount of computational time required, the L-REA model is concluded favourable for its use in optimisation and control of the coffee roasting process in the industry.

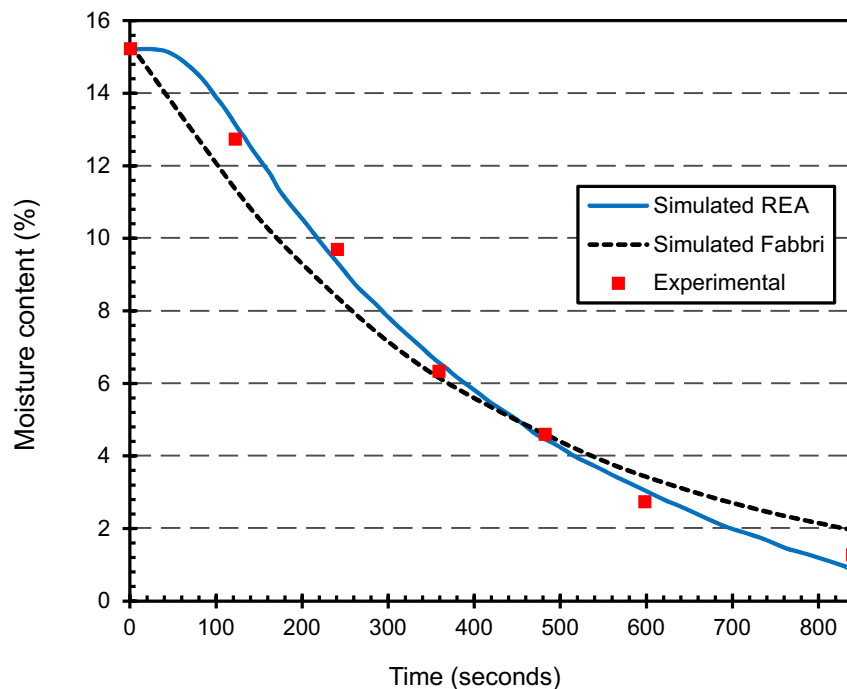


Figure 2.15: Simulated moisture content determined by Putranto & Chen (2012) compared to results obtained by Fabbri *et al.* (2011).

2.3.5 Comparison of models and applicability to this research

All the proposed models showed good correlation between the simulated and experimental results. Although the moisture loss model proposed by Schwartzberg (2002) overestimated the initial rate of water vaporisation during the roasting process, for the purpose of optimisation and control it is of little consequence, the model is well equipped to predict the final moisture content accurately, which can further assist in the determination of the roast degree.

As stated by Putranto & Chen (2012), the model used to simulate the roasting process needs to be robust, straightforward and accurate, and should require the least possible number of parameters determined by experiments. This is due to the fact that optimisation and control of the roasting process, is aimed at commercial roasters which are operated by an artisan roaster. For the fast implementation of optimisation and control, the proposed model should also not require immense amount of computational effort.

Although the model proposed by Fabbri *et al.* (2011) was found to be very accurate in predicting the bean temperature and moisture content, the computational effort required to simulate these results were immense due to three-dimensional nature of the geometry and it took up to an hour to obtain results. This is not ideal for the control of commercial roasters since real-time adjustments need to be made when correcting the roasting process.

With the exception of Schwartzberg (2002), all these models only predicted the bean temperature which was experimentally verified by thermocouples inserted into single beans to measure their temperature. This bean temperature cannot be verified during commercial roasting and therefore the models need to be adjusted to include the roast profile model proposed by Schwartzberg (2002). Although Heyd *et al.* (2007) did include a prediction of the outlet air temperature in the proposed model, which can quite easily be measured during real-time roasting, the temperature drop that occurs at the outlet of the roaster is greatly determined by the type of roaster. The temperature measured at the outlet is also dependent on the point where the measurement is taken and if the correct place is not used the measured temperature will differ quite a bit from the predicted temperature which can greatly influence optimisation and control.

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CHAPTER 3 – Experimental

Overview

In this chapter, the experimental methodology followed for the roasting experimental programme is described in detail. A description of the green coffee beans used during roasts is given in Section 3.1, followed by a thorough discussion in Section 3.2 regarding all the equipment used during experiments, as well as a detailed description of the various experimental setups. Finally, the experimental procedures that were followed are explained thoroughly in Section 3.3.

“I would rather suffer with coffee than be senseless.” – N. Bonaparte

3.1 Coffee beans

Arabica coffee beans originating from Brazil were used for roasting experiments and are shown in Figure 3.1. The coffee trees are grown between altitudes of 600 to 1000 meters in a tropical climate. The coffee cherries are then harvested with either the mechanical or strip picking method, during the June to September season. The dry natural method is used to process the harvested cherries and the final green coffee beans are classified as unwashed Arabica (Sevenoaks Trading, 2015).



Figure 3.1: Brazilian Arabica green beans.

The average properties of the green beans used during experiments are presented in Table 3.1.

Table 3.1: Physical properties of Arabica green coffee beans determined experimentally.

Average properties of green beans	
Weight (kg)	1.54×10^{-4}
Moisture content (wt%)	9.09
Longitudinal diameter (m)	9.23×10^{-3}
Equatorial diameter (m)	6.97×10^{-3}
Thickness (m)	3.56×10^{-3}

Measure values presented in Appendix A

3.2 Equipment and experimental setup

3.2.1 Coffee roaster

For the roasting experiments the Genio 6 Artisan coffee roaster, manufactured by Genio Intelligent Roasters (2016), was used and is exhibited in Figure 3.2. This roaster is based on a classic rotating drum roaster design, where the roasting chamber (roasting drum) is rotated over an open flame which is the source of heat throughout the entire system.

From Figure 3.2 it can be seen that the entire roaster system is connected to a control panel (1), from where all aspects of the roaster can be controlled. The source of the heat added to the system is established below the roasting drum (3), in the form of a burner fed with gas to sustain the flames (2). The gas flow to the burner can be adjusted to control the temperature of the air flowing into the drum.



Figure 3.2: Genio 6 Artisan roaster (adapted from Genio Intelligent Roasters, 2016).

The roasting drum, illustrated by Figure 3.3, rotates on an axis and has fins placed inside to continuously agitate the bean batch during roasting. The position of the burner relative to the drum can be adjusted, as well as the rotational speed of the drum, to control the amount of heat transferred via conduction. A draft is induced by the roasting fan (4) through the sides of the roaster over the open flames (2), passes through the perforated back-end of the drum, from where it comes into contact with the bean batch and transfers heat by means of convection. The amount of heat transferred by convection is controlled by the velocity of the air passing through the drum. The hot gas leaves the drum through the exhaust ducting (5).

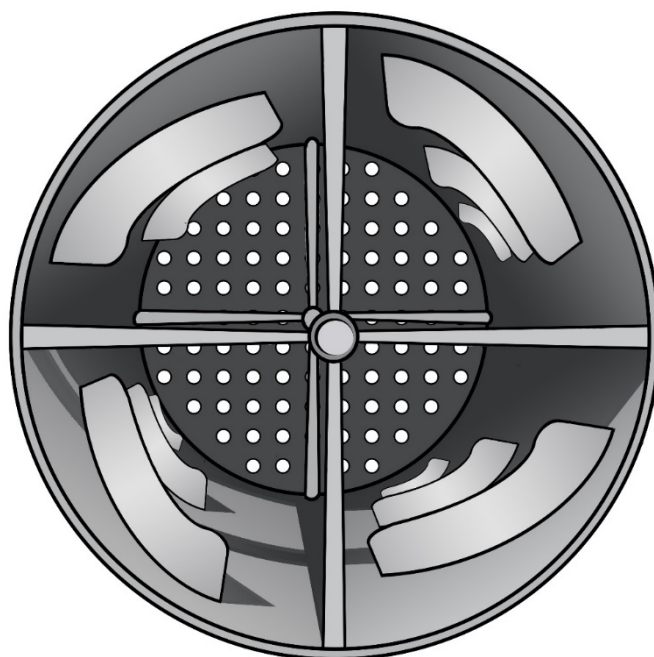


Figure 3.3: Illustration of the front view of the roasting drum (adapted from Rao, 2014).

Before the exhaust gas can be released into the atmosphere, it passes through a cyclone (6) where the particles in the gas stream (chaff and sometimes beans light enough to be carried by the gas stream) are separated from the gas and collected in a bin (7). The bin should be emptied regularly as the chaff collected poses a fire hazard, since it can be ignited when it comes into contact with a hot bean.

The bean batch enters the drum at the top of the roaster via a hopper (8), from where the beans can be released once the drum has reached the desired temperature. During the roast, the progress of the beans can be continuously evaluated as small samples of the batch can be collected through the sampling port (9) and extracted for either a visual inspection or other analyses like moisture content. After the desired degree of roast is reached, the beans are discharged and collected in the cooling bin (10) where the batch is cooled down to prevent over roasting. To ensure even cooling the bin has a stirring mechanism that agitates the beans as they are cooled. Air, at room temperature, is drawn through the bin by a cooling fan situated

inside the roaster, just below the bin (11). From the control panel the gas flow to the flames, the burner position relative to the drum, the rotational speed of the drum and the flow of the roasting air can be adjusted and controlled.

The roaster is controlled in three phases termed “Prime”, “Roast” and “Cool”. In order to ensure an even roasting, the drum is pre-heated before the beans are dropped into the drum. The roasting drum is prepared at a certain temperature (otherwise known as the start temperature of the roast profile) by starting the roaster in Prime phase. The desired roast start temperature is inserted on the control panel and the Prime phase is initiated. During this phase, adjustable parameters are controlled by the controller to reached the designated temperature and keep it there. Once the desired temperature is reached the Roast phase can be initiated. Once this phase is selected the automatic control over the adjustable parameters are released and changes to these parameters can be made during the process to help obtain the optimal roast. During this phase, the coffee beans are dropped into the drum and the roasting process begins. When the beans are discharged from the drum, after the desired degree of roast has been reached, the Cool-phase is started which activates the cooling fan and stirring mechanism, while cutting the flow of gas to the burner, extinguishing the flames.

The specifications of the Genio 6 roaster are tabulated in Table 3.2.

Table 3.2: Specifications of the roaster (adapted from Genio Intelligent Roasters, 2016).

Roaster specifications	
Bean capacity	Maximum 6 kg
Heat source	25kW gas burner
Gas source	Natural gas/LPG
Roasting fan	660 m ³ /hr at 1100 Pa
Cooling fan	1000 m ³ /hr at 1600 Pa
Heat transfer	Conduction and convection

3.2.2 Temperature measurement setup

During the roasting process, the temperature is measured by thermocouples at various points throughout the roaster, where some measurements are used to quantify the progression of the roast and others are used to determine the condition of the roasting air. As described in Section 2.2.4, the roast profile, which is used to quantify the roast progression, is measured with a thermocouple inserted into the bean batch inside the roasting drum and is demonstrated

by Figure 3.4 (a). Also depicted in Figure 3.4 (a) is the point at which the inlet air temperature is determined during the roasting process. These two thermocouples are installed by the manufacturers and are directly linked to the control panel.

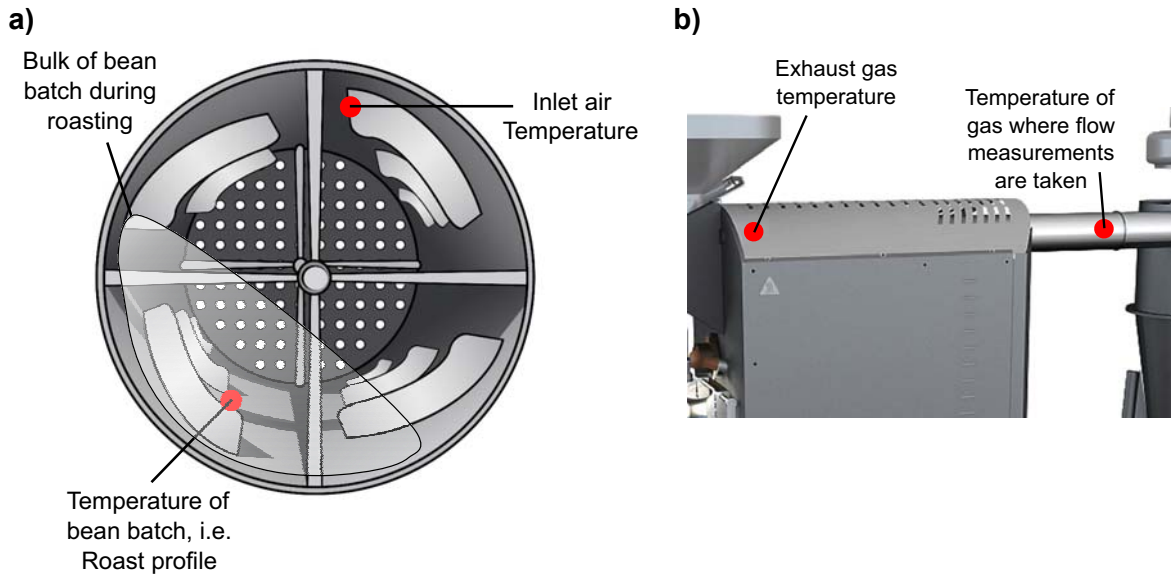


Figure 3.4: Illustration of where the temperature is measured in the a) drum and b) exhaust duct of the roaster.

In Figure 3.4 (b), the points where the temperatures are measured in the exhaust gas as it exits the drum and of the gas further down the line, are shown. Just as with the roast profile, the temperature development of the exhaust gas during the roasting process can be used to evaluate the roast development, as discussed in Section 2.3. The temperature of the exhaust gas measured further down the outlet ducting is used to help determine the gas flow through the system and is discussed in Section 3.3.7. These two thermocouples were post-manufacturing installations, as their value is significant for research purposes rather than for the artisanal coffee roaster.

All four thermocouples are connected to a data logger independent of the control panel, which logs the temperature of these four points continuously throughout the roasting process at one second intervals.

3.2.3 Green bean moisture increase setup

In order to assess the effects an increased green bean moisture content will have on the roast profile (which can indicate the behaviour of beans from other origins at different moisture contents), the green beans are steam treated to increase their moisture content.

Green beans are spread evenly over a stainless steel rack, with a perforated bottom, that is placed inside a stainless steel chamber. Steam is fed into the chamber at the bottom and allowed to travel through the bean batch, leaving through the open top of the chamber. The

bottom of the chamber is slanted with an outlet tube in the middle, to allow any steam that may condense against the rack and sides of the chamber to drain out. This is done to ensure that any accumulation of condensed water is released so that it cannot influence the flow of the steam.

After the beans have been steam treated, they are placed inside a container and allowed to rest for 2 days. This is done to ensure that the entire bean batch reaches the same moisture content and that any excess water on the surface of the beans, which was not absorbed, are allowed to evaporate.

3.2.4 Specifications of measuring instruments

Several instruments are used throughout the roasting experiments to determine the operating condition of the roasting air as well as the general properties of the green beans used during roasting. These instruments and their respective specifications are listed in Table 3.3.

Table 3.3: Instruments used for basic measurements.

Instrument	Application	Maximum	Resolution
Type K thermocouples	Measuring the temperature at several points in the roaster	1370 °C	0.025 °C
Pico technology USB TC-08 data logger	Directly logs temperature measurements to computer	Same as thermocouples connected	
Kern laboratory balances	To weigh the bean batch as well as the smaller samples	220 g 6000 g	0.1 mg 1 g
Delta Ohm HD 2301.0 Thermohygrometer	Used to determine the humidity of the hot roasting air	98 %RH at 180 °C	0.1 %RH
Kestrel 4000 Anemometer	To measure the velocity of air entering the roasting drum	60.0 m/s	0.1 m/s
NSK Micrometer	Determine the size of the green beans	25 mm	0.01 mm
Fluke 922 Airflow meter with pitot tube	Measure the gas flow through the system	99 999 m ³ /hr	1 m ³ /hr

3.3 Experimental procedures and analyses

3.3.1 Coffee bean moisture content

Experimental moisture content determination with whole roasted beans produces an overestimation of the moisture value, due to the weight loss of the entrapped gases within the bean that is released during the oven drying method of moisture content determination. Measuring the moisture content with ground beans delivers a better estimation of true moisture

content, because during grinding the entrapped gases are released as the beans are crushed (Clarke, 1987).

Determining the moisture content of coffee beans follows the rules for seed analysis according to Brazil (2009), based on a gravimetric method (De Oliveira *et al.*, 2016; Goneli *et al.*, 2013). First, the green and roasted beans are ground (Wang & Lim, 2012). The ground samples are weighed in an aluminium dish (the samples used are between 3 and 6 grams) and placed in a desiccator, to ensure the prepared samples does not lose or gain moisture from the environment. These samples are then placed in a laboratory oven, where it is dried at a constant temperature of 105 °C and for 24 hours. After the drying period is over, the samples are removed and placed in a desiccator to cool down. The ground samples are weighed again.

Equation 3.1 is used to determine the moisture content on a dry basis, where the sample weight before drying and after drying is used and the moisture content is calculated as a weight fraction (kg/kg).

$$X_b = \frac{m_{b,before} - m_{b,after}}{m_{b,after}} \quad \text{Equation 3.1}$$

In order to express the moisture content in terms of a weight percentage (wt%), Equation 3.2 is used.

$$X_b = \frac{m_{b,before} - m_{b,after}}{m_{b,after}} \times 100 \quad \text{Equation 3.2}$$

The average green bean moisture content is determined from 100 repeated experiments, while the roasted bean moisture content is determined from the samples extracted during roasting.

3.3.2 Roast loss

The roast loss is defined as the weight lost during roasting, due to volatile release, water evaporation and dry matter loss, and is determined by the difference between the weight of the green bean batch and the weight of the roasted beans after roasting. Equation 3.3 is used to calculate the roast loss percentage.

$$RL = \frac{m_{b,green} - m_{b,roast}}{m_{b,green}} \times 100 \quad \text{Equation 3.3}$$

3.3.3 First and second crack

During roasting the cracking/popping sound associated with the first and second crack can be heard. However due to the varied compositions of the bean batch (no one bean will be identical to another regarding its composition because of several factors – grown on different trees, level of ripeness when harvested, etc.) the cracking/popping is not heard all at once but rather

over a period of time, as all the beans in the batch reach that point. Some cracks/pops are heard fairly early, while others are only heard after the majority has already cracked/popped. For this reason, the beginning of the first and second crack is identified when a consistent cracking/popping sounds are heard.

3.3.4 General properties of green beans

To determine the average weight of the green beans, 100 green beans are weighed individually. The same procedure is followed for the moisture increased beans since the beans weight increases with the moisture content.

The green bean size is measured with a micrometre. The longitudinal and equatorial diameters, as well as the thickness of 100 green beans are measured (as demonstrated in Figure 3.5) to determine the average size of the beans. The same procedure is followed for the moisture increased beans since the beans swell in size when their moisture content are increased.

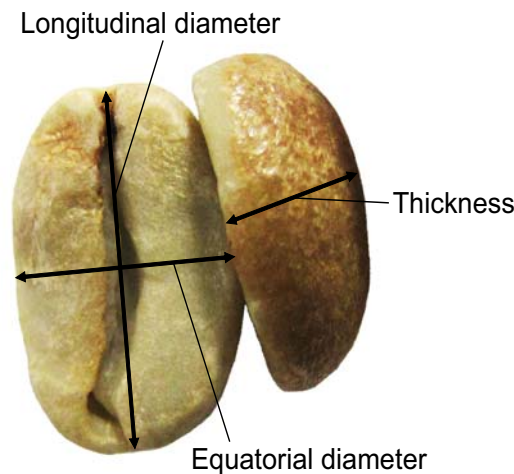


Figure 3.5: Demonstration of how the average bean size was determined.

3.3.5 Volume and density

Assuming that the shape of a coffee bean can be described by half a triaxial ellipsoid, the volume of an individual coffee bean can be calculated by Equation 3.4, with measurements taken of the equatorial and longitudinal diameter, as well as the thickness of a coffee bean (Dutra *et al.*, 2001; Franca *et al.*, 2005; Mendonca *et al.*, 2009).

$$V_b = \frac{2}{3}\pi abe \quad \text{Equation 3.4}$$

From Equation 3.4, the average density of coffee beans can be determined by the ratio of the average weight of an individual bean and the average calculated individual volume (Franca *et al.*, 2005; Mendonca *et al.*, 2009).

3.3.6 Air Velocity and gas mass flow rate

Due to the geometry of the air intake to the roaster system and consequently the drum, it is extremely difficult to measure the velocity of the air entering the drum during roasting. This is due to the fact that air is drawn in at both sides of the burner and during roasting the burner is turned on, making it hard to insert instruments at the point where the velocity should be measured. Therefore the roasting process is imitated by allowing the roasting fan to draw air through the system and the drum to rotate (at the same speed as during real roasting), however with the fuel gas to the burner being turned off. The exact same weight of green beans that is used during roasting is then dropped into the drum and the velocity is measured by holding the anemometer at the back of the drum directly in the path of the roasting air. This process is repeated 15 times to ensure that an accurate value is determined.

The rate at which the roasting air flows through the system is measured at the end of the exhaust gas ducting just before the cyclone, as shown in Figure 3.4 (b). The air flow rate is measured with a pitot tube attached to a manometer (Fluke 922 Airflow meter). The pitot tube is inserted into the pipe with its open tipped bend facing the oncoming gas stream and parallel with the duct wall. Due to the turbulent nature of the air flow through the duct, several measurements at various distances through the duct are taken and an average volumetric flow rate is determined. The points at which these measurements are taken are illustrated in Figure 3.6. The air flow measurements are repeated for 15 different roasts and are started 2 minutes into every roast.

To convert the average volumetric flow rate to an average mass flow rate, the air density at which the measurements are taken needs to be known. For this reason the temperature, as shown in Figure 3.4 (b), is also measured at this point. Using the equation proposed in Table 4.4, as described in Section 4.2, the average air density is then calculated, after which Equation 3.5 is used to calculate the average mass flow rate.

$$G = \frac{\dot{V} \times \rho_g}{3600} \quad \text{Equation 3.5}$$

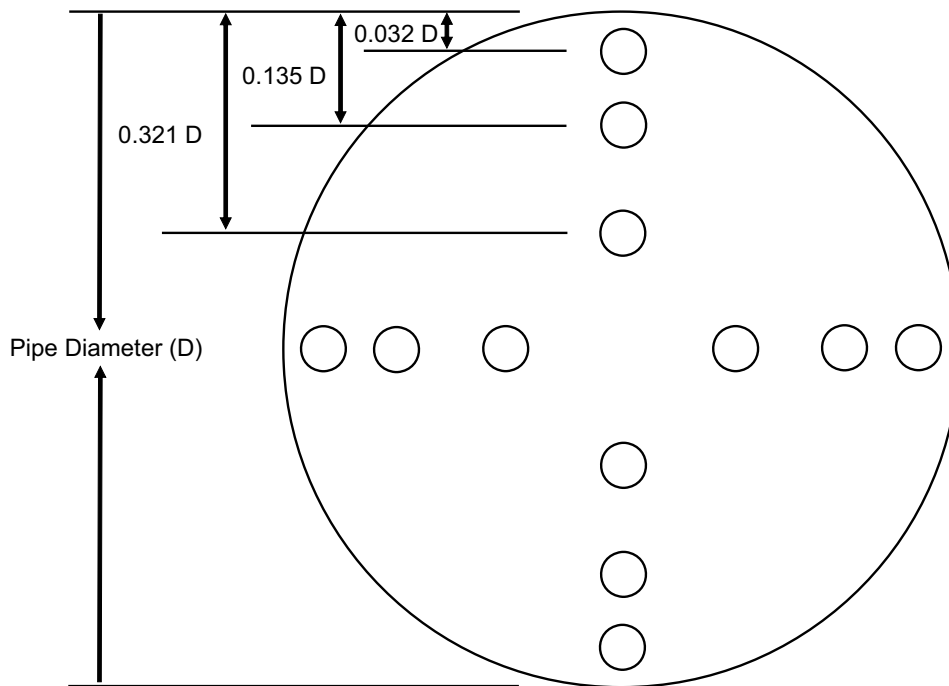


Figure 3.6: Points where measurements are taken inside the pipe (adapted from Fluke, 2006).

3.3.7 Moisture increase of green beans

The steam treatment setup, as described in Section 3.2.3, is used to increase the moisture content of the green coffee beans. The moisture content of the beans increases the longer they are exposed to the vapour. To produce a bean batch with a moisture content of 12.7, 13.3 and 14.5 wt%, the beans are exposed to the vapour for 10, 15 and 20 minutes respectively. In Table 3.4, the average properties of these green beans are presented.

Table 3.4: Average properties of moisture increased green beans determined experimentally.

Average properties of moisture increased green beans			
Weight (kg)	1.54×10^{-4}	1.57×10^{-4}	1.70×10^{-4}
Moisture content (wt%)	12.7	13.3	14.5
Longitudinal diameter (m)	9.54×10^{-3}	9.78×10^{-3}	1.03×10^{-2}
Equatorial diameter (m)	7.27×10^{-3}	7.52×10^{-3}	7.87×10^{-3}
Thickness (m)	4.12×10^{-3}	4.26×10^{-3}	4.36×10^{-3}

Measure values presented in Appendix A

3.3.8 Roast degree

The roast degree of the final roasted coffee is determined from the moisture content and the roast loss calculations carried out according to the descriptions in Sections 3.3.1 and 3.3.2 respectively. The values determined from these calculations are compared to literature values discussed in Sections 2.2.5.2 and 2.2.5.3. In conjunction with these calculated values the roast progression, as discussed in Section 2.2.5, is also used to determine the degree of roast.

3.3.9 Roasting procedure

Several parameters can be changed to influence the roasting process, from the drum rotation to the roasting time. In Table 3.5 the various changeable parameters are listed. Although all of these will influence the roasting process, only some are accounted for in the models proposed to simulate the roasting development (Section 4). Therefore some of the parameters are fixed to ensure consistent roasting.

The drum rotation will influence the mode of heat transfer, if the drum rotates slowly the beans will have a longer contact time with the drum and therefore more heat will be transferred due to conduction. The proposed models assume only convective heat transfer and as a result, the drum rotation is kept at its maximum to ensure convective heat transfer. The rotational speed of the drum is not accounted for in the proposed models.

The inlet air velocity is controlled by the fan speed drawing the air through the roaster. The Genio 6 artisan roaster combines the control for the drum rotation and fan speed, therefore adjusting it will influence both parameters. In the proposed models, the velocity of the inlet air will influence the calculated heat transfer coefficient and as a result the amount of heat transferred from the roasting air to the beans. During roasts the velocity of the inlet air is measured.

Another adjustable parameter is the position of the burner relative to the drum. The closer the burner is to the drum, the more heat will be absorbed by the drum due to its close proximity to the flames. As discussed above, only convective heat transfer are considered during modelling and as such the burner should be the farthest away from the drum than possible.

Table 3.5: Parameters that were changed during roasting.

Parameter	
Drum rotation	Fixed
Inlet air fan speed	Fixed
Position of burner relative to drum	Fixed
Gas flow to burner	Fixed
Roast start temperature	Varied
Roasting time	Varied

The amount of gas flow to the burner influences the temperature of the air flowing into the drum, however it also affects the amount of heat transferred to the drum since the burner is situated underneath the drum. Therefore the gas flow to the burner is fixed to a certain amount

so that mainly convective heat transfer can occur along with allowing for enough heat to be transferred to the roasting air.

Therefore, for all roasting experiments, the burner is kept the farthest distance away from the roasting drum and the gas flow to the burner is kept at 50 % flow. Also for every roast, the speed at which the drum rotates as well as the speed of the roasting fan is kept at its maximum.

The roast start temperature and the roasting time were varied to account for different roasting styles that different artisan roasters may implement. The reason for this is that a roast starting at 170 °C and roasted for 10 minutes can produce the same degree of roast coffee than a roast starting at 240 °C and lasting for 5 minutes. Therefore to assess the capability of the proposed models to simulated the roasting process at different start temperatures and roast durations, the roast start temperature is varied as well as the duration of the roasting process (for the varied time, the roast at different start temperatures are allowed to progress until after the second crack is reached to allow for the maximum accountability of the process). In Table 3.6, the roast temperature and time at which experiments are done, are listed.

As can be seen from Table 3.6, a variation in initial moisture content is also considered. This is done to investigate the capability of the proposed models to simulate the roasting process at different initial moisture content. The reason for this is to account for the fact that green coffee beans from various origins will not consist of the same initial moisture content.

Table 3.6: Roast experiments conducted.

Roast start temperature	Initial Moisture content	Roasting times	Repeats	Number of roasts
170, 180, 190, 200, 210, 220, 230 and 240 °C	9.09 wt%	10 minutes	3	24
170, 180, 190, 200, 210, 220, 230 and 240 °C	9.09 wt%	After second crack has been reached (10 to 15 minutes)	1	8
170, 190, 210, and 230 °C	12.7, 13.3 and 14.5 wt%	After second crack has been reached (11 to 17 minutes)	1	12

3.4 Experimental program

As discussed in Section 3.2.1, the roaster is first pre-heated in the Prime phase, to the desired roast start temperature. Once the Prime temperature has been reached the Roast phase is initiated and green beans are loaded into the hopper. The roast starts from the moment the beans are dropped into the roasting drum. The temperature at all four points (as described in

Section 3.2.2) are logged at one second intervals from the moment the roaster is turned on until after the roast is finished.

The first trial of roasting experiments is conducted with 4 kg green beans, roasted at roast start temperatures of 170 to 240 °C (in 10 °C intervals) for a roasting time of 10 minutes. Throughout the entire roast, bean samples are extracted at one minute intervals (starting from the beginning of the roast) to determine the average moisture content of the bean batch as the roast progresses. The times at which first and second crack is heard are noted and the bean batch is weighed after roasting to determine the roast loss. These roasting experiments are repeated three times for every temperature in order for an experimental error to be estimated.

The second trial of roasting experiments are conducted with 4 kg green beans, roasted at roast start temperatures of 170 to 240 °C (in 10 °C intervals), however this time the roast is allowed to progress beyond 10 minutes and is only stopped after the second crack has been reached. The same sampling and measurement procedure, as described for the first trial, is followed. These roasting experiments are only done once for every temperature.

The third trial of roasting experiments are conducted with 4 kg moisture increased green beans (moisture content starting at 12.74, 13.29, 14.54 wt%), roasted at roast start temperatures of 170 to 230 °C (in 20 °C intervals), these roasts are allowed to progress until after the second crack has been reached. The same sampling and measurement procedure, as described for the first trial, is followed. These roasting experiments are only done once for each increased moisture content at every temperature.

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CHAPTER 4 – Modelling of the roasting process

Overview

Chapter 4 focuses on the modelling of the roasting process. Here all relevant heat and mass transfer models are presented and explained in detail. All parameters and equations used during modelling are given as well as a description of how the models were implemented and solved. The solved models are verified through comparison with literature based results.

"The powers of a man's mind are directly proportioned to the quantity of coffee he drinks." – J. Mackintosh

4.1 Modelling Approach

As discussed in Section 2.3, various models have been proposed to model the roasting process. However, for the purpose of optimisation and control, the model chosen to be implemented needs to be accurate and robust. As well as having the ability to be implemented quickly and not requiring a great amount of computational effort (Putranto & Chen, 2012). Therefore the models proposed by Schwartzberg (2002) and Putranto & Chen (2012) are further investigated as to their suitability to model the roasting process.

The model proposed by Fabbri *et al.* (2011) was found to take a long time to solve and consequently not suitable for real-time control (as discussed in Section 2.3.5), however the modelling approach did deliver accurate results. Therefore a similar modelling approach is investigated (where the approach used by Hernández-Díaz *et al.* (2008) is also used for the moisture content determination) with the use of simplified geometry (assuming the coffee bean is in the shape of a sphere) and solved using the finite volume method.

4.1.1 Schwartzberg (2002) model

4.1.1.1 Bean temperature

During the roasting of coffee beans, heat is primarily transferred by convection from the hot roasting air to the bean batch (Φ_{gb}). Other forms of heat transfer will also take place during roasting. As the hot air flows through the roasting drum, heat is transferred to the exposed metal (Φ_{gm}). If enough heat is absorbed by the metal parts, it can transfer heat to the bean batch by means of conduction (Φ_{mb}) (Hernandez, 2002).

Studies conducted by Raemy (1981) and Raemy & Lambelet (1982) indicated that during the roasting of coffee beans (experimentally determined by using differential thermal analysis) exothermic reactions take place, generating a significant amount of heat (Φ_r) (Schwartzberg, 2002).

It is assumed that, as the beans are roasted, the moisture within the beans will diffuse to the surface and evaporate there. The evaporation that takes place at the surface of the beans is referred to as evaporative cooling. The energy necessary to support the evaporation comes from the beans, therefore as the surface evaporation takes place the beans will experience a decrease in temperature and as a result will experience heat loss due to evaporative cooling (Φ_{ev}) (Fabbri *et al.*, 2011; Incropera *et al.*, 2013).

From the above-mentioned, a heat balance over the beans in the roasting process will yield Equation 4.1.

$$m_b C p_b \frac{dT_b}{dt} = \Phi_{gb} - \Phi_{gm} + \Phi_{mb} + \Phi_r - \Phi_{ev} \quad \text{Equation 4.1}$$

The following assumptions are made to further simplify Equation 4.1:

- The heat transferred by the roasting air, otherwise named the rate of heat flow from the roasting air (Φ_{gb}) can be expressed by Equation 4.2 (Hernandez, 2002).

$$\Phi_{gb} = G_g C p_g [T_{g,i} - T_{g,o}] \quad \text{Equation 4.2}$$

- Hernandez (2002) assumed that the heat transferred from the roasting air to the metal (Φ_{gm}) will be significantly lower than the heat transferred to the beans by the roasting air (Φ_{gb}), because the entire roasting chamber was at a set temperature at the start of experiments. The same is assumed for the rotating drum roaster, for the entire drum is preheated before any roasting is done. Therefore the heat transferred to the metal (Φ_{gm}) is neglected.
- In a rotating drum roaster, the contact time between the hot metal and an individual bean is very small due to the rotation of the drum. Furthermore, the contact area of a single bean is very small ($A_b = 1.4 \times 10^{-4} \text{ m}^2$). From this it is assumed that the heat transferred due to conduction between the hot metal and the bean batch (Φ_{mb}) is negligible (Bottazzi *et al.*, 2012; Hernández *et al.*, 2007).
- The rate of heat flow from the heat generated by the exothermic reactions (Φ_r) can be expressed by Equation 4.3 (Hernandez, 2002).

$$\Phi_r = Q_r m_{b(d.b)} \quad \text{Equation 4.3}$$

- The energy related to the phase change of the moisture, as it evaporates from the surface of the beans, is the latent heat of vaporisation of water. Therefore the heat loss experienced by the beans due to evaporative cooling (Φ_{ev}) can be expressed by Equation 4.4 (Hernandez, 2002; Incropera *et al.*, 2013).

$$\Phi_r = \Delta H v \left(-\frac{dX_b}{dt} \right) m_{b(d.b)} \quad \text{Equation 4.4}$$

- During roasting, the weight of the coffee beans will change due to moisture loss, therefore the weight of the beans are considered with the change in moisture content and is expressed by Equation 4.5 (Hernandez, 2002).

$$m_b C p_b = m_{b(d.b)} (1 + X_b) C p_b \quad \text{Equation 4.5}$$

Following all the above-mentioned assumptions and substituting Equation 4.2 to Equation 4.5 into Equation 4.1, the temperature inside the bean can be expressed by Equation 4.6 (Schwartzberg, 2002).

$$\frac{dT_b}{dt} = \frac{G_g C p_g [T_{g,i} - T_{g,o}] + m_{b(d.b)} \left(Q_r + \Delta H v \frac{dX_b}{dt} \right)}{m_{b(d.b)} (1 + X_b) C p_b} \quad \text{Equation 4.6}$$

According to Schwartzberg (2002), the roasting air temperature changes significantly as it passes through the roaster. During roasting, only a portion of the beans are in direct contact with the air flow at any given time, and their change in temperature are relatively small as a small amount of air passes through. In order to model the air temperature change it is assumed that the air flow through the drum is uniform (the velocity of the air is also assumed to be uniform as it passes through the bean batch) and travels in a single direction, that there is no accumulation of air in the drum and that all thermophysical properties of the air stays constant relative to the air temperature (Hernandez, 2002). Neglecting any other heat transfer than the convective heat transfer between the hot air and the bean batch, an air temperature balance of the air, as it passes through the drum, can then be expressed by Equation 4.7 (Schwartzberg, 2002).

$$-G_g C p_g \frac{dT_g}{dZ} = h e \left(\frac{dA_b}{dZ} \right) [T_g - T_b] \quad \text{Equation 4.7}$$

During roasting, the bean temperature (T_b) and surface area (A_b) will vary from bean to bean at any given time. Therefore these values will be determined from the averages of the entire bean batch. The effective heat transfer coefficient (he) is used in Equation 4.7, instead of directly using the calculated heat transfer coefficient, and is calculated using Equation 4.11 (Schwartzberg, 2002). Integrating Equation 4.7 between the temperatures of the air entering the drum and the air leaving the drum ($T_{g,i}$ and $T_{g,o}$ respectively), and rearranging, Equation 4.8 is obtained.

$$\int_{T_{g,i}}^{T_{g,o}} \frac{1}{(T_g - T_b)} dT_g = - \frac{he A_b}{G_g C p_g} \quad \text{Equation 4.8}$$

Equation 4.8 can be further simplified to Equation 4.9.

$$(T_{g,o} - T_b) = (T_{g,i} - T_b) \left(\exp \left[- \frac{he A_b}{G_g C p_g} \right] \right) \quad \text{Equation 4.9}$$

Rearranging Equation 4.9 to be in terms of the difference between the temperatures of the air entering the drum and the air leaving the drum, Equation 4.10 is acquired. During modelling

Equation 4.10 can then be substituted into Equation 4.6 to help determine the bean temperature.

$$(T_{g,i} - T_{g,o}) = (T_{g,i} - T_b) \left(1 - \exp \left[-\frac{heA_b}{G_g C p_g} \right] \right) \quad \text{Equation 4.10}$$

According to Schwartzberg (2002), the effective heat transfer coefficient (he) can be determined using Equation 4.11.

$$he = \frac{h}{1 + 0.3Bi} \quad \text{Equation 4.11}$$

Schwartzberg (2002) modelled the exothermic heat generation based on the assumptions that the rate of the heat generated is relative to the reactions that produce the heat, and that the rate at which these reactions take place is proportional to the concentration of the reactants (that is assumed to be consumed during these reactions) which is governed by an Arrhenius type equation. Schwartzberg (2002) proposed Equation 4.12 to determine the rate at which these exothermic reactions produce heat (Q_r).

$$Q_r = Ar \cdot \exp \left[\frac{-\Delta E}{R(T_b)} \right] \left(\frac{Het - He}{Het} \right) \quad \text{Equation 4.12}$$

This proposed equation, along with the constant values used during modelling, is based on experimental data obtained by Raemy (1981) and Raemy & Lambelet (1982). Table 4.1 presents the constant values that were estimated by Schwartzberg (2002) to be used in conjunction with Equation 4.12 to determine the heat generated by the exothermic reaction.

Table 4.1: Constant values used during modelling (taken from Schwartzberg, 2002).

Constant values used for modelling		
Ar	$116\,200 \times 10^3$	W/kg
$\Delta E/R$	5 500	K
Het	232×10^3	J/kg
ΔHv	2790×10^3	J/kg

Equation 4.13 is used to determine the heat produced thus far during roasting at any given time (Schwartzberg, 2002).

$$He = \sum Q_r \cdot \Delta t \quad \text{Equation 4.13}$$

4.1.1.2 Moisture content

Schwartzberg (2002) proposed Equation 4.14, a semi-empirical equation, to model the moisture loss that takes place during roasting. This model only accounts for the evaporation of the initial moisture content of the bean and does not take into consideration water formation that may occur during the roasting reactions. It was assumed that the moisture loss was diffusively controlled and that an Arrhenius type equation governed the temperature dependency of the diffusion coefficient (Bottazzi *et al.*, 2012; Schwartzberg, 2002).

$$-\frac{dX_b}{dt} = \frac{4.32 \times 10^9 \cdot X_b^2}{(d_b \times 10^3)^2} \exp \left[\frac{-9889}{T_b} \right] \quad \text{Equation 4.14}$$

This equation is based on corrected moisture loss data which were obtained from experimental roasting data that were adjusted to exclude any moisture increase due to reaction based water formation (this was done by subtracting any estimated increase in moisture from the obtained data).

4.1.1.3 Roast profile

As previously discussed, the roast profile is one of the primary parameters by which the roasting process is controlled and it is of great importance to be able to reproduce a desired roast profile for overall repeatable product quality. Therefore Schwartzberg (2002) proposed Equation 4.15, to predict the roast profile from the simulated bean temperature. This can greatly help to see how various parameters can influence the bean temperature and thereby the roast profile, subsequently assisting in optimising the roasting process to obtain a desired roast profile from which a superior quality product can be produced repeatedly.

$$\frac{dT_{rp}}{dt} = K(T_b - T_{rp}) \quad \text{Equation 4.15}$$

The value of the roast profile constant (K) was determined to be 0.016. This was done through regression from experimental results presented by Schwartzberg (2002) (see Appendix F).

4.1.2 Putranto & Chen (2012) model

4.1.2.1 Bean temperature

Putranto & Chen (2012) proposed Equation 4.16 to determine the bean temperature during roasting, which is derived similarly to Equation 4.6 proposed by Schwartzberg (2002). However, Putranto & Chen (2012) disregarded any heat transfer that may occur between the roasting air and metal of the drum and subsequently between the metal and the bean batch, as well as heat generated by the exothermic roasting reaction. Putranto & Chen (2012)

assumed that heat is only transferred from the roasting air to the beans and that during roasting, heat loss occurs due to evaporative cooling.

$$\frac{dT_b}{dt} = \frac{hA_b(T_{g,i} - T_b) + m_{b(d.b)} \frac{dX_b}{dt} \Delta H_v}{m_{b(d.b)}(1 + X_b)Cp_b} \quad \text{Equation 4.16}$$

4.1.2.2 Moisture content

Putranto & Chen (2012) proposed a moisture loss model which uses the L-REA to estimate the moisture content during the roasting process. The L-REA is thusly named because the mass balance used for modelling the moisture loss is expressed by a lumped parameter ordinary differential equation. This approach is started by expressing the rate at which water evaporates from the surface of the bean by Equation 4.17 (Chen, 2008).

$$\frac{dm_b}{dt} = -kA_b(p_{v,s} - p_{v,g,i}) \quad \text{Equation 4.17}$$

However, as the drying continues it can begin to be hindered by the structure of the coffee bean (moisture at the centre of the bean must first diffuse to the surface before it can evaporate). Therefore the drying rate of the wet solid can be expressed in terms of the dry mass of the material ($m_{b(d.b)}$), as shown by Equation 4.18 (Chen, 2008).

$$m_{b(d.b)} \frac{dX_b}{dt} = -kA_b(p_{v,s} - p_{v,g,i}) \quad \text{Equation 4.18}$$

The surface vapour concentration ($p_{v,s}$) can be determined from the saturated vapour concentration by using Equation 4.19 (Putranto & Chen, 2012), where the activation energy (ΔE) represents the difficulty that exists in extracting moisture at various drying stages and is dependent on the moisture content of the coffee beans (Chen, 2008).

$$p_{v,s} = \exp\left(\frac{-\Delta E}{RT_b}\right) p_{v,sat} \quad \text{Equation 4.19}$$

Putranto & Chen (2012) proposed Equation 4.20 to determine the saturated vapour concentration at various bean temperatures, which was estimated based on established data summarised by Keey (1992).

$$p_{v,sat} = 4.844 \times 10^{-9} (T_b - 273.15)^4 - 4.844 \times 10^{-9} (T_b - 273.15)^3 + 3.683 (T_b - 273.15)^2 - 2.837 (T_b - 273.15) + 0.988 \quad \text{Equation 4.20}$$

Combining Equation 4.19 and Equation 4.20, and substituting it into Equation 4.18, the moisture loss of the coffee beans, using the L-REA, can then be expressed by Equation 4.21 (Putranto & Chen, 2012).

$$\frac{dX_b}{dt} = -kA_b \left[\exp\left(\frac{-\Delta E}{RT_b}\right) p_{sat} - p_g \right] \frac{1}{m_{b(d.b)}} \quad \text{Equation 4.21}$$

Rearranging the parameter in Equation 4.21, the activation energy can be determined by Equation 4.22. The activation energy is determined from one accurate drying experiment. Putranto & Chen (2012) used experimental data determined by Burmester & Eggers (2010) for the drying of green coffee beans at 55 °C and 10 %RH.

$$\Delta E = -RT_b \ln \left[\frac{-m_{b(d.b)} \frac{dX_b}{dt} \frac{1}{kA_b} + p_g}{p_{sat}} \right] \quad \text{Equation 4.22}$$

The activation energy's dependency on moisture content can be related to the relative activation energy ($\frac{\Delta E}{\Delta E_{eq}}$), which is determined by using Equation 4.23 (Putranto & Chen, 2012).

The internal behaviour of the coffee beans during roasting, is basically described by the relative activation energy and the energy generated from Equation 4.23 can be applied for other roasting conditions on condition that the same material, with a similar initial moisture content, is being roasted (Putranto & Chen, 2012).

$$\frac{\Delta E}{\Delta E_{eq}} = f(X_b - X_{eq}) \quad \text{Equation 4.23}$$

The equilibrium activation energy is determined by Equation 4.24, which represent the maximum activation energy that can be attained under specific roasting air temperature and relative humidity. The equilibrium moisture content corresponds to the temperature and relative humidity of the roasting air, which is correlated to one another by means of the equilibrium isotherm (Putranto & Chen, 2012).

$$\Delta E_{eq} = -RT_{g,i} \ln(RH_{g,i}) \quad \text{Equation 4.24}$$

Using the activation energy determined with Equation 4.22 and the experimental results obtained by Burmester & Eggers (2010), and the equilibrium activation energy determined with Equation 4.24, the relative activation energy is determined. The relative activation energy curve is created using Equation 4.23. A curve fit is done on the relative activation energy curve using the least squares method, from which a mathematical expression is obtained to describe the relative activation energy related to the moisture content. Putranto & Chen (2012) found a good fit between the experimental and fitted results ($R^2 = 0.997$), and subsequently proposed Equation 4.25 to be used in conjunction with Equation 4.21 to determine the moisture loss during the roasting process.

$$\frac{\Delta E}{\Delta E_{eq}} = -1.683(X_b - X_{eq})^3 + 3.683(X_b - X_{eq})^3 - 2.837(X_b - X_{eq})^3 + 0.988 \quad \text{Equation 4.25}$$

4.1.3 Finite volume heat transfer model for a sphere

A model based on a simplified geometry is proposed to determine the bean temperature during roasting. The coffee bean is assumed to be in the shape of a sphere and that the coffee bean properties will vary radially within the sphere (Basile & Kikic, 2009; Heyd *et al.*, 2007). From these assumptions, the general form of the heat equation for unsteady heat transfer in a one-dimensional sphere, shown by Equation 4.26, is proposed to be used to determine the bean temperature during the coffee roasting process (Knudsen *et al.*, 1997).

$$\frac{\partial}{\partial t}(\rho C_p T) = \frac{1}{r^2} \left[\frac{\partial}{\partial r} \left(\lambda r^2 \frac{\partial T}{\partial r} \right) \right] + \frac{\partial q}{\partial t} \quad \text{Equation 4.26}$$

The proposed partial differential equation is solved using the finite volume method, as described by Versteeg & Malalasekera (2007), where the sphere is divided into control volumes. The partial differential equation is then integrated over the specified control volumes, from where it is discretised to obtain a system of ordinary differential equations that can be solved simultaneously.

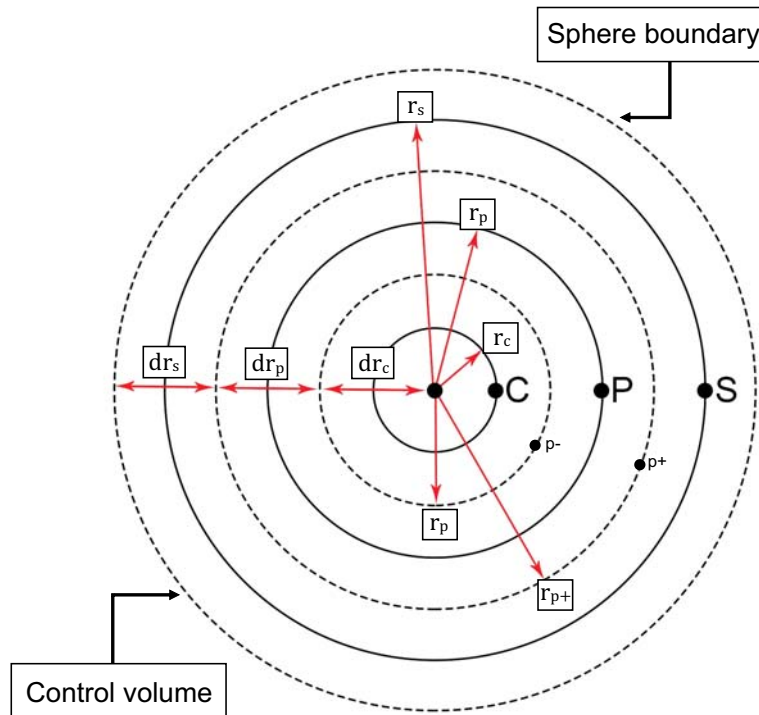


Figure 4.1: Schematic representation of a sphere divided into equally spaced control volumes

First, a one-dimensional sphere is considered. This sphere is then divided into three layers (namely the centre layer – C, the middle layer - P, and the surface layer - S) with equally

spaced control volumes (which is based on the control volume length), as illustrated in Figure 4.1 (Versteeg & Malalasekera, 2007). For this sphere, it is assumed that heat transfer occurs by convection from the hot roasting air to the surface of the sphere and then by conduction through the sphere to the centre.

Next follows the integration of Equation 4.26 over a control volume as shown in Equation 4.27.

$$\int_{CV} \frac{\partial}{\partial t} (\rho C_p T) dV = \int_{CV} \frac{1}{r^2} \left[\frac{\partial}{\partial r} \left(\lambda r^2 \frac{\partial T}{\partial r} \right) \right] dV + \int_{CV} \frac{\partial q}{\partial t} dV \quad \text{Equation 4.27}$$

Equation 4.27 can be further simplified by writing it in terms of the boundaries of a typical control volume, which in this case is the control volume surrounding the middle layer. Doing this will yield Equation 4.28 (Versteeg & Malalasekera, 2007).

$$\int_{p-}^{p+} \frac{\partial}{\partial t} (\rho C_p T) dV = \int_{p-}^{p+} \frac{1}{r^2} \left[\frac{\partial}{\partial r} \left(\lambda r^2 \frac{\partial T}{\partial r} \right) \right] dV + \int_{p-}^{p+} \frac{\partial q}{\partial t} dV \quad \text{Equation 4.28}$$

Equation 4.28 can now be further simplified into Equation 4.29 (Versteeg & Malalasekera, 2007).

$$\frac{\partial}{\partial t} (\rho C_p T) [\Delta V]_{p-}^{p+} = \left(\left[\lambda A \frac{\partial T}{\partial r} \right]_{p+} - \left[\lambda A \frac{\partial T}{\partial r} \right]_{p-} \right) + \dot{q} [\Delta V]_{p-}^{p+} \quad \text{Equation 4.29}$$

The volume, with regards to the middle layer ($[\Delta V]_{p-}^{p+}$), can now be expressed in terms of the geometric formula to determine the volume of a sphere, as shown in Table 4.2. However, it can be further simplified to be more easily calculated from the radius of the layer and the thickness of the control volumes, as expressed by Equation 4.30.

$$[\Delta V]_{p-}^{p+} = \frac{4}{3} \pi [r_{p+}^3 - r_{p-}^3] = \frac{4}{3} \pi [(r_p + 0.5dr_p)^3 - (r_p - 0.5dr_p)^3] \quad \text{Equation 4.30}$$

Substituting the geometric formula to determine the area of a sphere, as shown in Table 4.2, Equation 4.29 can now be replaced by Equation 4.31.

Table 4.2: Geometric formulas for a sphere (taken from Stewart, 2009).

Geometric formulas for a sphere	
Volume	$V = \frac{4}{3} \pi r^3$
Area	$A = 4\pi r^2$

$$\frac{\partial}{\partial t}(\rho C_p T)[\Delta V]_{p-}^{p+} = \left(\left[\lambda 4\pi r^2 \frac{\partial T}{\partial r} \right]_{p+} - \left[\lambda 4\pi r^2 \frac{\partial T}{\partial r} \right]_{p-} \right) + \dot{q}([\Delta V]_{p-}^{p+}) \quad \text{Equation 4.31}$$

For a sphere, the heat conduction through the boundary layer can be written in terms of the thermal resistance, as shown in Equation 4.32, when integrating over the control volume. Where the general equation for thermal resistance for a spherical shell is expressed in Equation 4.33, where r_1 represents the inner radius of the spherical shell and r_2 the outer radius (Incropera *et al.*, 2013).

$$\lambda A \frac{\partial T}{\partial r} = \frac{1}{Rt} \Delta T \quad \text{Equation 4.32}$$

$$Rt = \frac{1}{4\pi\lambda} \left(\frac{1}{r_1} - \frac{1}{r_2} \right) \quad \text{Equation 4.33}$$

If it is assumed that the temperature of one layer will prevail for the entire control volume, the heat conduction that travels from the surface layer to the middle layer, at the control volume boundary at their interface ($p +$), can now be expressed in terms of thermal resistance. The same can be done for the heat conduction that travels from the middle layer to the centre layer, at the control volume boundary at their interface ($p -$) (Versteeg & Malalasekera, 2007).

Integrating and implementing the thermal resistance equation, the heat conduction through the two control volume boundaries ($p +$ and $p -$), can now be written as shown in Equation 4.34 and Equation 4.35, respectively.

$$\left[\lambda 4\pi r^2 \frac{\partial T}{\partial r} \right]_{p+} = \frac{1}{Rt_S} (T_S - T_P) \quad \text{Equation 4.34}$$

$$\left[\lambda 4\pi r^2 \frac{\partial T}{\partial r} \right]_{p-} = \frac{1}{Rt_C} (T_P - T_C) \quad \text{Equation 4.35}$$

Where the thermal resistance across the control volume can be determined by Equation 4.36 and Equation 4.37 (le Grange, 2012).

$$Rt_S = \frac{1}{8\pi} \left(\frac{dr_P}{\lambda_P r_P (r_P + 0.5dr_P)} + \frac{dr_S}{\lambda_S r_S (r_S - 0.5dr_S)} \right) \quad \text{Equation 4.36}$$

$$Rt_C = \frac{1}{8\pi} \left(\frac{dr_C}{\lambda_C r_C (r_C + 0.5dr_C)} + \frac{dr_P}{\lambda_P r_P (r_P - 0.5dr_P)} \right) \quad \text{Equation 4.37}$$

Therefore the bean temperature at the middle layer can be determined by Equation 4.38.

$$\frac{\partial T_P}{\partial t} = \frac{\frac{1}{Rt_S}(T_S - T_P) - \frac{1}{Rt_C}(T_P - T_C) + \dot{q}([\Delta V]_{p-}^{p+})}{(\rho_b C p_b)[\Delta V]_{p-}^{p+}} \quad \text{Equation 4.38}$$

The same procedure can be followed for the centre layer, however, only conduction from the centre layer to the middle layers takes place, therefore the volume of the control volume over the centre layer can be calculated with Equation 4.39.

$$[\Delta V]_{C-}^{C+} = \frac{4}{3}\pi[r_{C+}^3] = \frac{4}{3}\pi[(r_C + 0.5dr_C)^3] \quad \text{Equation 4.39}$$

The thermal resistance between the two layers can be determined the same way as Equation 4.36, however it should be in terms of the centre layers radius. Therefore the thermal resistance between the centre and middle layer (Rt_P) can be expressed by Equation 4.40 (le Grange, 2012).

$$Rt_P = \frac{1}{8\pi} \left(\frac{dr_C}{\lambda_C r_C (r_C + 0.5dr_C)} + \frac{dr_P}{\lambda_P r_P (r_P - 0.5dr_P)} \right) \quad \text{Equation 4.40}$$

Therefore the bean temperature at the centre layer can be determined by Equation 4.41.

$$\frac{\partial T_C}{\partial t} = \frac{\frac{1}{Rt_P}(T_P - T_C) + \dot{q}([\Delta V]_{C-}^{C+})}{(\rho_b C p_b)[\Delta V]_{C-}^{C+}} \quad \text{Equation 4.41}$$

At the surface of the sphere, heat is transferred from the hot roasting air to the surface by means of convection. Therefore the same procedure can be followed as with the middle layer, only the surface layer will have a boundary condition at the interface between the hot roasting air and the sphere. After integrating over the control volume at the surface layer, Equation 4.42 can be found.

$$\frac{\partial}{\partial t}(\rho C p T)[\Delta V]_{S-}^{S+} = \left(\left[\lambda A \frac{\partial T}{\partial r} \right]_{s+} - \left[\lambda A \frac{\partial T}{\partial r} \right]_{s-} \right) + \dot{q}([\Delta V]_{S-}^{S+}) \quad \text{Equation 4.42}$$

The volume of the control volume over the surface layer can be determined by Equation 4.43, using the same method as with the middle layer.

$$[\Delta V]_{S-}^{S+} = \frac{4}{3}\pi[r_{S+}^3 - r_{S-}^3] = \frac{4}{3}\pi[(r_S + 0.5dr_S)^3 - (r_S - 0.5dr_S)^3] \quad \text{Equation 4.43}$$

Since heat transfer due to convection takes place at the interface between the surface of the bean and the hot roasting air, i.e. at the boundary of the surface layer ($s +$), and accounting for the effects of evaporative cooling, the boundary condition can be given by Equation 4.44 (Fabbri *et al.*, 2011; Heyd *et al.*, 2007; Incropera *et al.*, 2013).

$$-\lambda \frac{\partial T}{\partial r} = h(T_s - T_g) - m_{b(d.b)} \frac{dX}{dt} \Delta H_v \quad \text{Equation 4.44}$$

The thermal resistance between the surface and middle layer can be calculated with Equation 4.36. It is assumed that the environment temperature is known and therefore the bean temperature at the surface layer can be determined by Equation 4.45.

$$\frac{\partial T_s}{\partial t} = \frac{hA(T_g - T_s) + m_{b(d.b)} \frac{dX}{dt} \Delta H_v - \frac{1}{Rt_s}(T_s - T_p) + \dot{q}([\Delta V]_{s-}^{s+})}{(\rho_b C p_b)[\Delta V]_{s-}^{s+}} \quad \text{Equation 4.45}$$

4.1.4 Hernández-Díaz *et al.* (2008) moisture content model

Ruiz-Lopez *et al.* (2011) proposed Equation 4.46 to model the moisture loss of a hemispherical solid during a drying process. This equation was derived from the unsteady mass transfer equation for moisture diffusion in a sphere.

$$\frac{dX_b}{dt} = -kmS(X_b - X_{eq}) \quad \text{Equation 4.46}$$

The internal mass transfer coefficient (km) is calculated by using Equation 4.47. The internal mass transfer coefficient is related to the slope of an average drying curve (Λ) that represents the drying (or roasting) process, which needs to be determined experimentally (Ruiz-Lopez *et al.*, 2011).

$$km = \frac{\Lambda^2 D_b}{L^2 S} \quad \text{Equation 4.47}$$

Using Equation 4.46 and Equation 4.47, Hernández-Díaz *et al.* (2008) established Equation 4.48 from drying experiments conducted on 20 coffee beans placed in a drying chamber. The beans were dried with air temperatures ranging from 40 °C to 60 °C, for a maximum of 5 hours.

$$\frac{dX_b}{dt} = -\frac{12.3 D_b}{L^2} (X_b - X_{eq}) \quad \text{Equation 4.48}$$

Hernández-Díaz *et al.* (2008) suggested Equation 4.49, to determine the moisture diffusivity in coffee beans. Equation 4.49 was formulated by fitting the diffusivities calculated from experimental runs to an Arrhenius type equation.

$$D_b = \exp\left(2.7085 - \frac{66856.4}{RT} + 1.74 \frac{X_b}{X_{b,i}}\right) \quad \text{Equation 4.49}$$

4.2 Heat and mass transfer coefficients

The heat transfer coefficients depend on the conditions at the interface between the fluid and the material. These conditions are significantly influenced by the surface geometry of the material, the transport and thermodynamic properties of the fluid and the nature of the fluid movement (Incropera *et al.*, 2013). These coefficients can readily be determined by the use of the dimensionless parameter, the Nusselt number.

For the roasting of coffee beans in hot air, it is assumed that the shape of the beans can be correlated to that of a sphere (Basile & Kikic, 2009; Burmester & Eggers, 2010; Fabbri *et al.*, 2011). Therefore the Ranz-Marshall correlation is used to determine the heat transfer coefficient, given by Equation 4.50 (Basile & Kikic, 2009; Clarke, 1987; Hernández *et al.*, 2007).

$$Nu = 2 + 0.6 Re^{\frac{1}{2}} Pr^{\frac{1}{3}} \quad \text{Equation 4.50}$$

Considering the different parameters that can influence the heat transfer coefficient, the calculated heat transfer coefficient can range between 14 W/m²·K and 75 W/m²·K (Eggers & Pietsch, 2001). Nagaraju *et al.* (1997) reported a heat transfer coefficient ranging between 10 W/m²·K and 22 W/m²·K for roasting in a spouted bed roaster. Where Basile & Kikic (2009) found a value of 26.7 W/m²·K.

The dimensionless groups used for the calculations of the heat transfer coefficient is presented in Table 4.3.

Table 4.3: Dimensionless groups used during heat transfer coefficient calculations, (adapted from Incropera *et al.*, 2013; Nilnont *et al.*, 2012).

Dimensionless group	Formula
Biot number	$Bi = \frac{hd_b}{\lambda_b}$
Nusselt number	$Nu = \frac{hd_b}{\lambda_g}$
Prandtl number	$Pr = \frac{Cp_g \mu_g}{\lambda_g}$
Reynolds number	$Re = \frac{v_g d_b \rho_g}{\mu_g}$

The mass transfer coefficient is calculated by Equation 4.51, which was proposed by Fabbri *et al.* (2011) in terms of moisture concentration inside the coffee bean and further simplified to be expressed in terms of moisture content by the coffee bean density proposed by Putranto & Chen (2012).

$$k = \frac{5.09 \times 10^{-4}}{224.46X_b + 7.6308} \quad \text{Equation 4.51}$$

Ramirez-Martinez *et al.* (2010) reported that, when calculated, the mass transfer coefficient will range between 3.3×10^{-4} m/s and 4.8×10^{-5} m/s.

As mentioned, the heat and mass transfer coefficients depend on the transport and thermodynamic properties of the fluid. In the case of coffee roasting with hot air, these properties will include the density, heat capacity, viscosity and thermal conductivity of air. Various sources have reported values for these properties, however they are temperature dependent as these properties can change significantly with the change of temperature. Using the values supplied by Incropera *et al.* (2013), temperature dependent equation were formulated, as shown in Table 4.4 to determine these properties at various roasting air temperatures (see Appendix C for a detailed description of how these equations were determined).

Table 4.4: Equations used to determine the thermophysical properties of drying air at various temperatures.

Thermophysical properties of drying air	
Density of drying air	$\rho_g = 353.34 \times T_g^{-1.002}$
Heat capacity of drying air	$Cp_g = 5.3091 \times 10^{-17}[T_g^6] - 4.1550 \times 10^{-13}[T_g^5] + 1.3621 \times 10^{-9}[T_g^4] - 2.3267 \times 10^{-6}[T_g^3] + 2.1034 \times 10^{-3}[T_g^2] - 7.2075 \times 10^{-1}[T_g] + 1.0839 \times 10^3$
Viscosity of drying air	$\mu_g = 1.2184 \times 10^{-24}[T_g^6] - 8.1123 \times 10^{-21}[T_g^5] + 1.6089 \times 10^{-17}[T_g^4] + 1.1460 \times 10^{-15}[T_g^3] - 3.9733 \times 10^{-11}[T_g^2] + 7.1226 \times 10^{-8}[T_g] + 4.8855 \times 10^{-7}$
Thermal conductivity of drying air	$\lambda_g = 1.3819 \times 10^{-20}[T_g^6] - 9.1506 \times 10^{-17}[T_g^5] + 2.2342 \times 10^{-13}[T_g^4] - 2.2872 \times 10^{-10}[T_g^3] + 6.8867 \times 10^{-8}[T_g^2] + 8.0128 \times 10^{-5}[T_g] + 7.6694 \times 10^{-4}$

4.3 Properties of coffee beans

4.3.1 Heat capacity of coffee beans

Various formulae have been published for the determination of coffee bean heat capacity and in Table 4.5 these formulae are presented. In order to determine which formula will be best

suited to use during modelling, the heat capacity of coffee beans is calculated with experimental data obtained by Fabbri *et al.* (2011). As can be seen from Table 4.5, the formula proposed by Schwartzberg (2002) is not only dependent on moisture content but also on the bean temperature. The corresponding bean temperature is therefore used in combination with the moisture content to determine the coffee bean heat capacity in this case. (Appendix D contains the experimental data used in these calculations).

Table 4.5: Heat capacity of coffee beans.

Heat capacity of coffee beans	
(Schwartzberg, 2002)	$Cp_b = \frac{1.099 + 0.0070(T_b - 273.15) + 5.0X_b}{(1 + X_b)} \times 10^3$
(Putranto & Chen, 2012)	$Cp_b = \left(1.674 + 2.51 \frac{X_b}{1 + X_b}\right) \times 10^3$
(Hernández-Díaz <i>et al.</i> , 2008)	$Cp_b = 1652.2 + 5835 \frac{X_b}{1 + X_b}$
(Fabbri <i>et al.</i> , 2011)	$Cp_b = \frac{0.0116c_b + 0.062}{(5 \times 10^{-9}c_b + 6 \times 10^{-8}) \cdot (78.845c_b + 1723)}$

In Figure 4.2, the heat capacity for coffee beans using the formulae presented in Table 4.5 is shown. As is apparent from the first look, the heat capacity calculated from the formula proposed by Fabbri *et al.* (2011) does not feature on the graph. This is due to the fact that while the other calculated capacities ranged between 1.6 kJ/kg·K and 3 kJ/kg·K, the heat capacity from Fabbri *et al.* (2011) did not even go above 70 J/kg·K, which was in direct conflict with the experimental values reported by Fabbri *et al.* (2011). For a moisture content ranging from 15 to 1 wt%, Fabbri *et al.* (2011) reported that the heat capacity will range between 1.2 kJ/kg·K and 1.7 kJ/kg·K.

According to Eggers & Pietsch (2001), the heat capacity of green coffee beans will increase from 2.8 to 6 kJ/kg·K as the beans temperature increases from 25 to 85 °C, and then decrease as the beans temperature increases, reaching a heat capacity of 2 kJ/kg·K at 210 °C. If the bean's temperature exceeds 210 °C, which is believed to be when strong exothermic reactions take place, the heat capacity will decline further. For already roasted coffee beans, a heat capacity ranges from 2 to 2.5 kJ/kg·K as the temperature increases from 25 to 210 °C.

Chandrasekar & Viswanathan (1999) found that the heat capacity increases as the moisture content of the coffee beans increases. This is reflected in the proposed formulas from Putranto & Chen (2012) and Hernández-Díaz *et al.* (2008), for the calculated heat capacity decreases as the moisture content decreases. However, as shown by Eggers & Pietsch (2001), the heat capacity will also be dependent on the temperature of the bean. From this it is concluded that

the formula proposed by Schwartzberg (2002) may estimate a more accurate heat capacity for the coffee beans, for as observed by Eggers & Pietsch (2001), the initial heat capacity increases as the initial bean temperature increases, then later on it decreases as the temperature became even higher. The influence of the formulas proposed by Putranto & Chen (2012) and Hernández-Díaz *et al.* (2008) will be further investigated when implemented in the heat and mass transfer model, which will be discussed in Section 4.6.

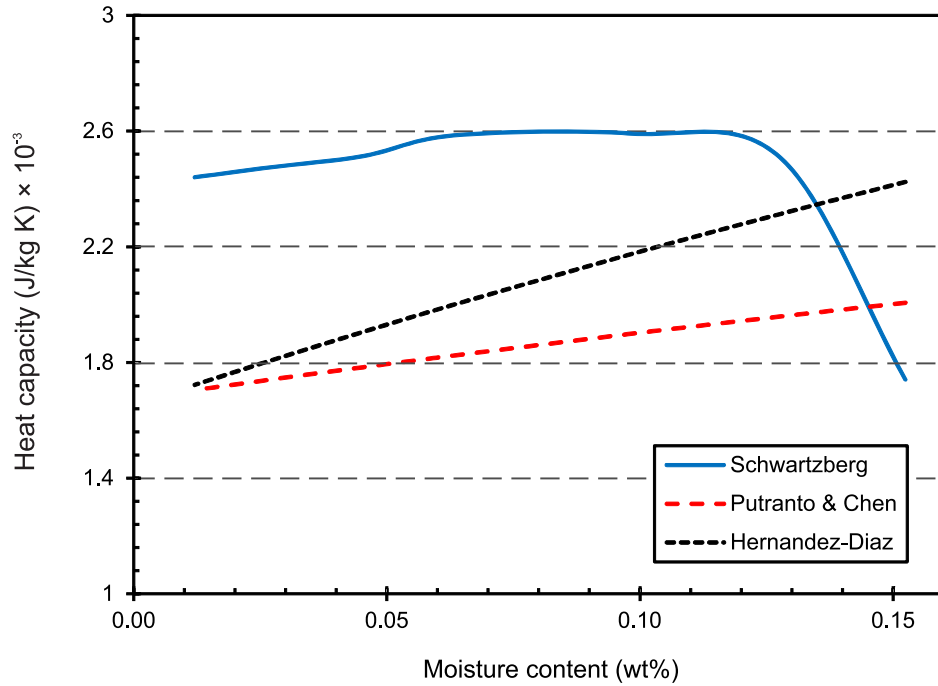


Figure 4.2: Heat capacity of coffee beans.

4.3.2 Thermal conductivity of coffee beans

Various formulas have been reported for the determination of the thermal conductivity of coffee beans and these are presented in Table 4.6.

Table 4.6: Thermal conductivity of coffee beans.

Thermal conductivity of coffee beans	
(Hernandez, 2002)	$\lambda_b = 0.356 + 0.139X_b$
(Hernández-Díaz <i>et al.</i> , 2008)	$\lambda_b = 0.49 - 0.443\exp^{-0.206X_b}$
(Fabbri <i>et al.</i> , 2011)	$\lambda_b = 0.0116c_b + 0.062$

In order to determine which formula will be best suited to use during modelling, the thermal conductivity of coffee beans is calculated with experimental data obtained by Fabbri *et al.* (2011). The thermal conductivity determined from the experimental data is presented in Figure 4.3.

As can be seen in Figure 4.3., the thermal conductivity calculated from the formula proposed by Fabbri *et al.* (2011) does not feature on the graph. This is due to the fact that, while the other calculated conductivities ranged between 0.04 W/m·K and 0.4 W/m·K, the thermal conductivity calculated from Fabbri *et al.* (2011) ranges between 5 W/m·K and 65 W/m·K, which is significantly higher than the experimental values reported by Fabbri *et al.* (2011). For a moisture content ranging from 15 to 1 wt%, Fabbri *et al.* (2011) reported that the thermal conductivity will range between 0.07 W/m·K and 0.15 W/m·K.

According to Sivetz & Desrosier (1979), the thermal conductivity of coffee beans behave similar to that of wood, and that it depends greatly on its moisture content. By using this analogy, Eggers & Pietsch (2001) found that an average value of 0.173 W/m·K will exist for the thermal conductivity of coffee beans. However, Burmester & Eggers (2010) reported the thermal conductivity for coffee beans to range from 0.2 W/m·K and 0.4 W/m·K, for coffee bean moisture content ranging from 7 to 30 wt%. Therefore the formulas proposed by Hernandez (2002) and Hernández-Díaz *et al.* (2008) will be considered during modelling, and will be evaluated when implemented in the heat and mass transfer model, which will be discussed in Section 4.6.

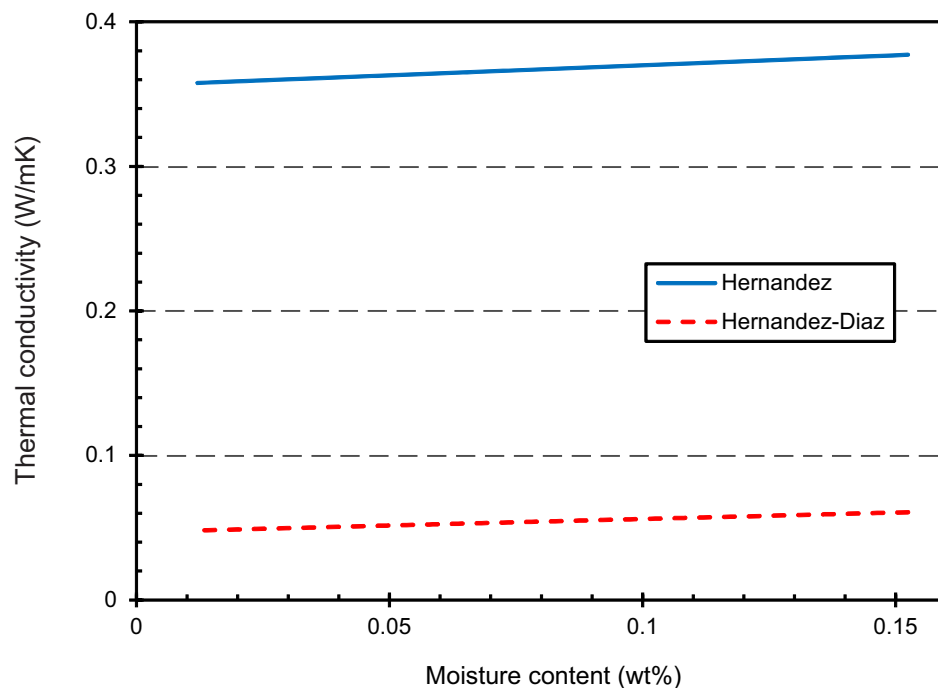


Figure 4.3: Thermal conductivity of coffee beans.

4.3.3 Density of coffee beans

Assuming that the shape of a coffee bean can be described by half a triaxial ellipsoid, the volume of an individual coffee bean can be calculated by Equation 3.4, with measurements taken of the equatorial and longitudinal diameters as well as the thickness of a coffee bean, as illustrated in Figure 3.5 (Dutra *et al.*, 2001; Franca *et al.*, 2005; Mendonca *et al.*, 2009).

$$V_b = \frac{2}{3}\pi a b e \quad \text{Equation 4.52}$$

From Equation 3.4, the average density of coffee beans can be determined by the ratio of the weight of the beans and the sum of their calculated volume (Franca *et al.*, 2005; Mendonca *et al.*, 2009).

It has been reported that the bean density of green beans will range between 1200 kg/m³ and 1300 kg/m³, and that of roasted beans will be between 450 kg/m³ and 850 kg/m³ (Franca *et al.*, 2005; Mendonca *et al.*, 2009).

Fabbri *et al.* (2011) proposed Equation 4.53 to determine the bean density as a function of its moisture content, however, this equation was soon disregarded from just preliminary calculations as the initial bean moisture concentration reported by Fabbri *et al.* (2011) provided an unrealistic value (i.e. for an initial moisture concentration of 5400 mol/m³ the bean density calculated was 427 × 10³ kg/m³).

$$\rho_b = 78.845c_b + 1723 \quad \text{Equation 4.53}$$

For the purpose of modelling, Putranto & Chen (2012) assumed an average bean density of 635.9 kg/m³.

4.3.4 Surface area of coffee beans

Hernandez (2002) suggested Equation 4.54 to calculate the surface area of an individual coffee bean, based on the measurements of the equatorial and longitudinal diameter of the bean.

$$A_b = \frac{\pi}{4}ab + \frac{\pi}{4}\left[b^2 + ab\left(\frac{\arcsin(\varepsilon)}{\varepsilon}\right)\right] \text{ where } \varepsilon = \frac{\sqrt{a^2 - b^2}}{a} \quad \text{Equation 4.54}$$

The surface area of the entire bean batch is calculated with the number of beans in the batch (i.e. the total weight of the batch divided by the average weight of an individual bean) and the average surface area calculated for an individual coffee bean using Equation 4.54 (Bottazzi *et al.*, 2012; Hernández-Díaz *et al.*, 2008).

4.3.5 Equilibrium moisture content

The equilibrium moisture content of coffee beans at the specific roasting air initial conditions (inlet temperature and relative humidity of the roasting air) are determined by the formula given by Equation 4.55, where the water activity being used is calculated from the relative humidity of the air (Berbert *et al.*, 1995).

$$X_{eq} = 1.1281 \left[\frac{-\ln(1 - a_w)}{((T_g - 273.15) + 40.535)} \right]^{0.5405} \quad \text{Equation 4.55}$$

4.4 Statistical performance parameters

In order to evaluate the goodness of fit of the proposed models to experimental data the following statistical performance parameters are determined, i.e. the statistical coefficient of determination, mean relative error and the root mean square error (Gómez-De La Cruz *et al.*, 2015; Taitano & Singh, 2013; Toğrul & Pehlivan, 2003).

The coefficient of determination, R^2 , is determined by linear regression and the values determined should range between 0 and 1. A value of R^2 exceeding 0.7, is generally accepted to indicate that a model can predict the tendency of the experimental values to a good extent (Devore & Farnum, 2005; Ramsaroop & Persad, 2012).

The root mean square error, RMSE, is determined by Equation 4.56, and the smaller the value of the RMSE, the closer will the predicted values be to the experimentally obtained values (Gómez-De La Cruz *et al.*, 2015; Putranto *et al.*, 2010).

$$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^N (Y_{exp,i} - Y_{pre,i})^2} \quad \text{Equation 4.56}$$

The mean relative error, MRE, is determined by Equation 4.57, and the smaller the value determined, the better the model fits the experimental results (De Oliveira *et al.*, 2016; Taitano & Singh, 2013).

$$MRE = \frac{100}{N} \sum_{i=1}^N \frac{|Y_{exp,i} - Y_{pre,i}|}{Y_{exp,i}} \quad \text{Equation 4.57}$$

However, it should be noted that when using the MRE a higher percentage error will be found for models that overestimate the predicted values. This is due to the fact that the MRE have a heavier penalty for positive errors than negative errors, and in fact has a limit of 100 % when values are underestimated, but there is no limit when overestimation occurs (Hyndman & Koehler, 2006; Shcherbakov *et al.*, 2013).

4.5 Solving the models

The proposed models are all implemented in Simulink® 8.7 (2016). The ordinary differential equations are set up and subsequently solved, using the solver ode3, from initial values (bean temperature, moisture content and roast profile start temperature) at the beginning of the roast

time (roast begins at 0 s) at time intervals of one second until the end of the roast. In Appendix E, the implemented models in Simulink® 8.7 (2016) are presented.

For the pebble model, it is assumed that all layers of the bean start from the same initial bean temperature. The bean temperature for all three layers are determined and then the average thereof determined to describe the entire bean temperature. Moisture content is determined using the average bean temperature.

4.6 Verification of bean temperature with literature results

Due to the nature of the roaster used during roasting experiments (rotating drum), the bean temperature cannot be measured during roasting. Therefore, the three postulated models are implemented and the bean temperature is verified using literature-based results.

Heyd *et al.* (2007) conducted roasting experiments with a spouted bed roaster. A 100 grams batch of green Arabica coffee beans (harvested in Colombia) was roasted for 10 minutes at an inlet air temperature range of 180 to 250 °C. The initial values and model parameters needed to simulate the roasting process at these conditions are presented in Table 4.7, and the modelled bean temperature and moisture content are compared to experimental results obtained by Heyd *et al.* (2007), for roasting at inlet air temperature of 210 °C and 250 °C.

Table 4.7: Literature values used for model verification (adapted from Hernández *et al.*, 2007; Heyd *et al.*, 2007).

Parameter	Value
A_b	0.08 m ²
d_b	6.6×10^{-3} m
G_g	0.02 kg/s
$m_{b(d.b)}$	91.8×10^{-3} kg d.b
$RH_{g,i}$	0.1 %
$T_{b,i}$	20 °C
$T_{g,i}$	210, 250 °C
t	600 s
v_g	0.2 m/s
$X_{b,i}$	0.082 kg/kg d.b.
X_{eq}	1.36, 1.26×10^{-3} kg/kg d.b.

4.6.1 Schwartzberg (2002)

The Schwartzberg (2002) model discussed in Section 4.1.1 is implemented as described in Section 4.5, with the model parameters required for simulation taken from Table 4.7. As discussed previously, four equations have been obtained to calculate the heat capacity of the

coffee beans (Table 4.5) where only the three identified in Section 4.3.1 are used during modelling. The same applies for the thermal conductivity of coffee beans, where three equations were acquired (Table 4.6), but only the two identified in Section 4.3.2 will be further investigated during modelling.

In Table 4.8, the combination in which these equations were implemented during modelling is illustrated.

Table 4.8: Combination of heat capacity and thermal conductivity of coffee beans used during modelling.

Heat capacity	Thermal conductivity	Model name
(Schwartzberg, 2002)	(Hernandez, 2002)	Sch_Cp1_λ1
	(Hernández-Díaz <i>et al.</i> , 2008)	Sch_Cp1_λ2
(Putranto & Chen, 2012)	(Hernandez, 2002)	Sch_Cp2_λ1
	(Hernández-Díaz <i>et al.</i> , 2008)	Sch_Cp2_λ2
(Hernández-Díaz <i>et al.</i> , 2008)	(Hernandez, 2002)	Sch_Cp3_λ1
	(Hernández-Díaz <i>et al.</i> , 2008)	Sch_Cp3_λ2

Using the above-mentioned parameters and equations, the bean temperature and moisture content were simulated for the given roasting conditions. In Table 4.9 and Table 4.10, the statistical fitting efficiency parameters are tabulated (as discussed in Section 4.7) for the simulated bean temperature and moisture content respectively.

Table 4.9: Statistical fitting efficiency parameters determination for predicted bean temperature at 210 °C and 250 °C.

Model	210 °C			250 °C		
	R ²	RSME	MRE	R ²	RSME	MRE
Sch_Cp1_λ1	0.954	9.74	6.41	0.949	14.5	8.29
Sch_Cp1_λ2	0.901	19.7	9.40	0.893	28.5	12.5
Sch_Cp2_λ1	0.974	8.21	5.78	0.973	9.81	6.18
Sch_Cp2_λ2	0.913	17.0	7.95	0.918	21.7	8.94
Sch_Cp3_λ1	0.959	9.94	6.19	0.960	12.1	6.41
Sch_Cp3_λ2	0.886	21.2	9.69	0.890	27.0	10.4

The modelling done using the thermal conductivity formula proposed by Hernández-Díaz *et al.* (2008) (λ2), showed a marked difference to those conducted with Hernandez (2002) (λ1), as can be seen from the statistical fitting efficiency parameters calculated and presented in Table 4.9 and Table 4.10. This is due to the fact that Schwartzberg (2002) proposed that an

effective heat transfer coefficient that is related to the Biot number (Equation 4.11), should be used for determining the heat transferred to the coffee beans. Since the heat transfer coefficient (obtained as discussed in Section 4.2) determined for all six combinations were between 31 to 32 W/m²·K, the effective heat transfer coefficient decreased from about 29 to 19 W/m²·K when using the lower thermal conductivity proposed by Hernández-Díaz *et al.* (2008). This decrease initiated a decrease in simulated heat transfer which directly influenced the bean temperature and moisture content.

A slight difference in accuracy of the bean temperature predicted results (Table 4.9) can be observed for the inlet air temperatures. For all combinations of heat capacity and thermal conductivity, the values predicted for the lower inlet air temperature fitted better to experimental results than that of the higher inlet air temperature. This could indicate a sensitivity to the inlet air temperature showing that the higher this temperature the less accurate the model becomes.

Table 4.10: Statistical fitting efficiency parameters determination for predicted moisture content at 210 °C and 250 °C.

Model	210 °C			250 °C		
	R ²	RSME	MRE	R ²	RSME	MRE
Sch_Cp1_λ1	0.933	1.16	22.3	0.654	2.37	72.8
Sch_Cp1_λ2	0.845	1.92	47.2	0.471	3.28	125
Sch_Cp2_λ1	0.955	0.90	14.7	0.749	1.93	52.3
Sch_Cp2_λ2	0.876	1.58	34.5	0.535	2.85	92.9
Sch_Cp3_λ1	0.937	1.08	18.7	0.683	2.21	61.9
Sch_Cp3_λ2	0.840	1.83	42.6	0.470	3.16	111

A significant difference in accuracy was observed for the moisture content predicted results (Table 4.10) determined for the different inlet air temperatures. At 250 °C, only the model Sch_Cp2_λ1 could be identified to have a fairly good fit compared to the experimental results ($R^2 > 0.7$, with the lowest determined values for RSME (1.93 wt%) and MRE (52.3 %)). From this, it can be concluded that accuracy of the moisture loss model proposed by Schwartzberg (2002) is significantly influenced by the inlet air temperature.

From the values presented in Table 4.9 and Table 4.10, it was determined that, excluding the model combination that include the lower thermal conductivity (thermal conductivity formula proposed by Hernández-Díaz *et al.* (2008), the Schwartzberg (2002) model can adequately predict the bean temperature and moisture content of coffee beans during the given roasting conditions, with the accuracy of the moisture content prediction decreasing somewhat with

higher temperatures which concludes a slight overestimation of the moisture content during roasting (as can be seen from Figure 4.5).

It was concluded that the best fit to experimental results was obtained from the combination of heat capacity and thermal conductivity parameters given by Putranto & Chen (2012) and Hernandez (2002) respectively (model Sch_Cp2_λ1). The bean temperature and moisture content results obtained from this model compared to the experimental results obtained by Heyd *et al.* (2007) are presented in Figure 4.4 and Figure 4.5.

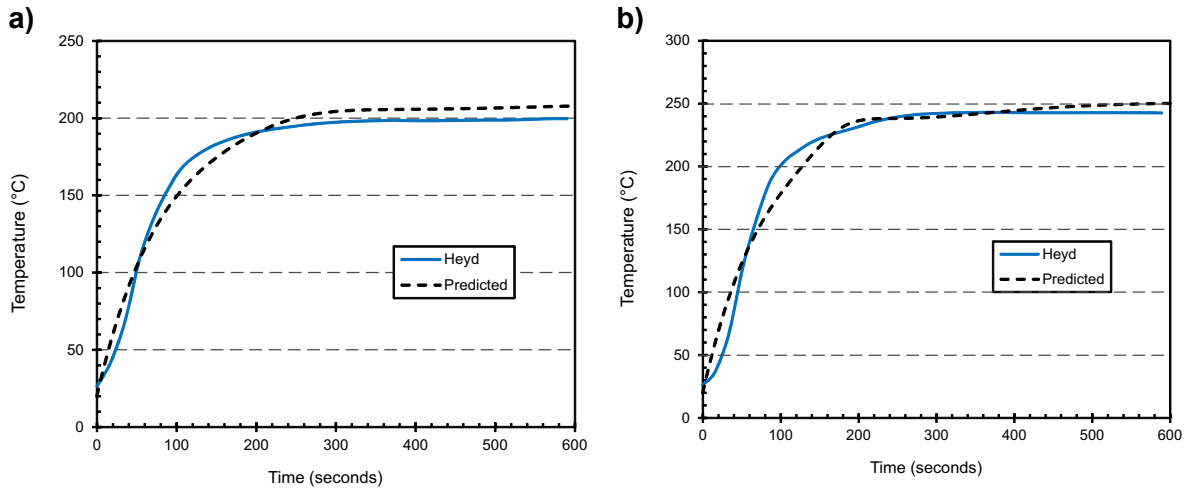


Figure 4.4: Best model fit (Sch_Cp2_λ1) to bean temperature obtained from literature data at a) 210 °C inlet air temperature and b) 250 °C inlet air temperature.

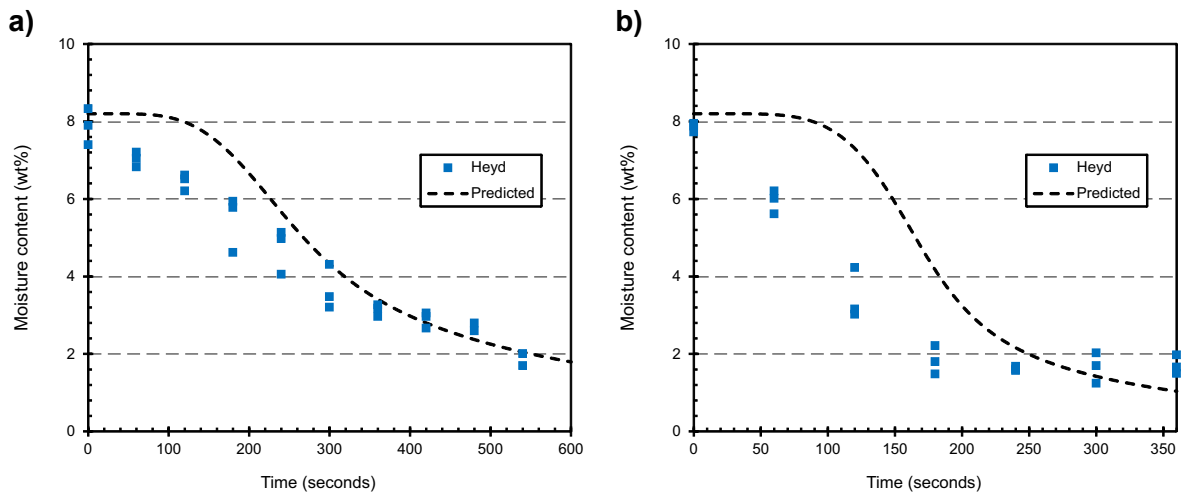


Figure 4.5: Best model fit (Sch_Cp2_λ1) to moisture content obtained from literature data at a) 210 °C inlet air temperature and b) 250 °C inlet air temperature.

The equation proposed by Schwartzberg (2002) to determine the moisture content of coffee beans during roasting (Equation 4.14) was further investigated. This was done to see what effect a difference in inlet air temperature and initial moisture content will have on the accuracy of the model. Using the values presented in Table 4.7, the roasting process was first simulated for varying initial moisture content values at a constant inlet air temperature and then for varying inlet air temperatures at a constant initial moisture content.

The effect these variations in values had on the moisture content during the roasting process can be seen in Figure 4.6. According to the simulated model, the higher the initial moisture content the faster the moisture will evaporate, as can be seen in Figure 4.6 (a). This behaviour is verified by Figure 4.7, however not as drastically as the simulated results implied. According to the simulated results for a batch consisting of 18 wt% initial moisture content, the beans will lose the bulk of their moisture in a span of 100 s which seems rather unrealistic. Compared to results obtained by Schenker (2000) (shown in Figure 4.7), the results obtained from the moisture loss model for varying initial moisture content will decrease in accuracy as the initial moisture content increases.

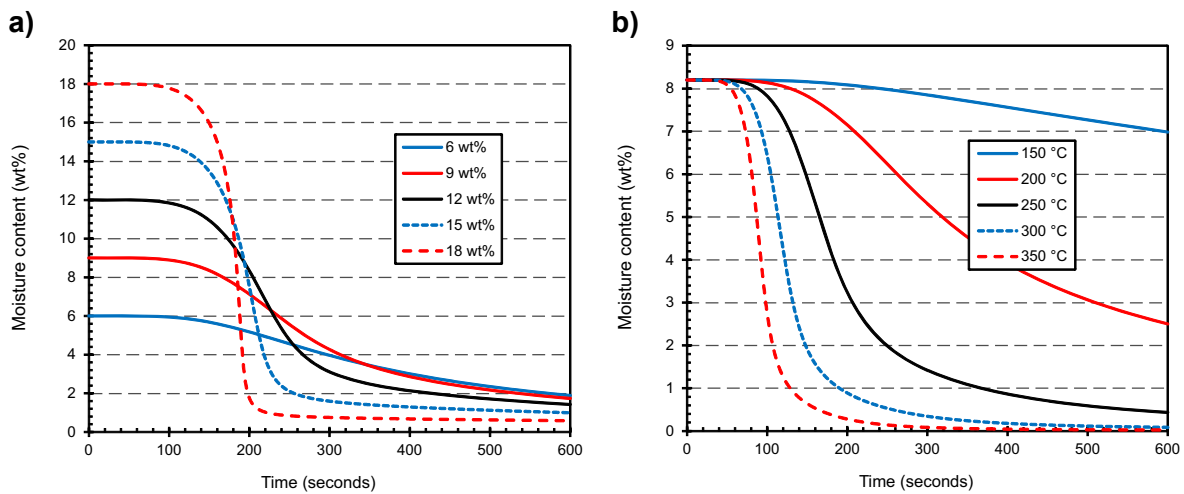


Figure 4.6: Predicted moisture content a) at varying initial moisture content (inlet air temperature constant) and b) at varying inlet air temperature (initial moisture content constant).

This can be attributed to the empirical nature of the equations. The values reported to be used as constants during modelling were fitted to correspond to a set of experimental results and the increase in initial moisture content falls outside of the range used to determine the experimental data. Therefore, this moisture content equation can only be accurately used for a certain range of initial moisture contents.

The effect the inlet air temperature has on the moisture content during the roasting process is presented in Figure 4.6 (b), showing that the higher the inlet air temperature, the faster the moisture will evaporate from the beans (Burmester & Eggers, 2010). For the higher temperatures the rate of moisture loss is fairly fast. Again, at the higher temperature the bulk of the moisture is lost in less than 100 s. From this, it is determined that the moisture loss model proposed by Schwartzberg (2002) can only be used with certain accuracy when a roasting process with low initial moisture content and inlet air temperature is considered.

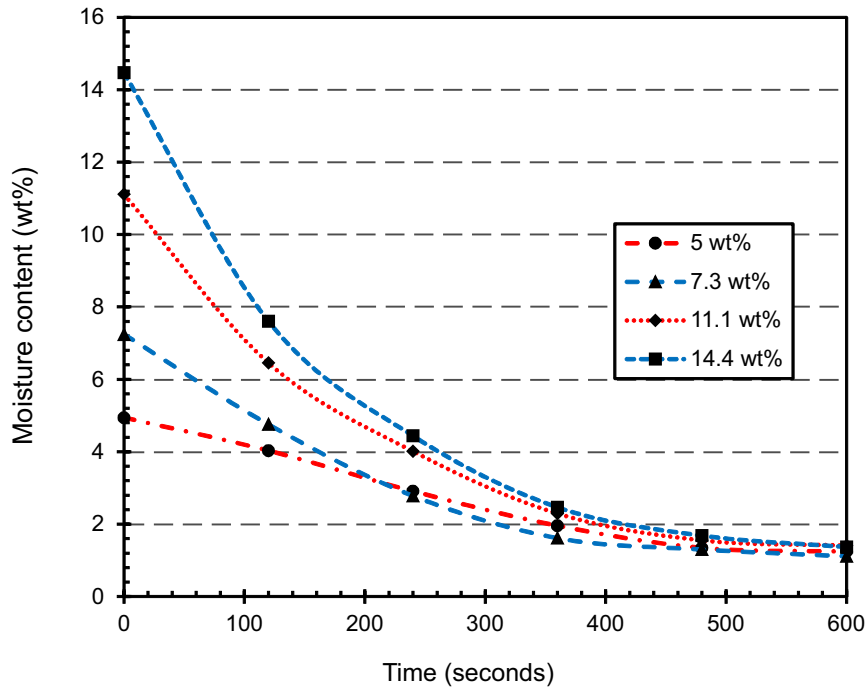


Figure 4.7: Experimental moisture content at inlet air temperature of 260 °C for varying initial moisture content, adapted from (Schenker, 2000).

The effect the modelled moisture loss during the roasting process has on the bean temperature is displayed in Figure 4.8. The deviation observed in the bean temperature (peak in bean temperature between 150 s and 300 s during the roasting process) can be attributed to the fast moisture loss described in Figure 4.6 (a), which overestimates the bean temperature with over 100 °C. The moisture content and temperature of the bean directly influence one another, as a decrease in the moisture content leads to an increase in the bean temperature. This is attributed to less energy being consumed for evaporation of the moisture as the moisture content decreases, leading to the heat being applied to heat the bean and thus increase its temperature (Burmester & Eggers, 2010).

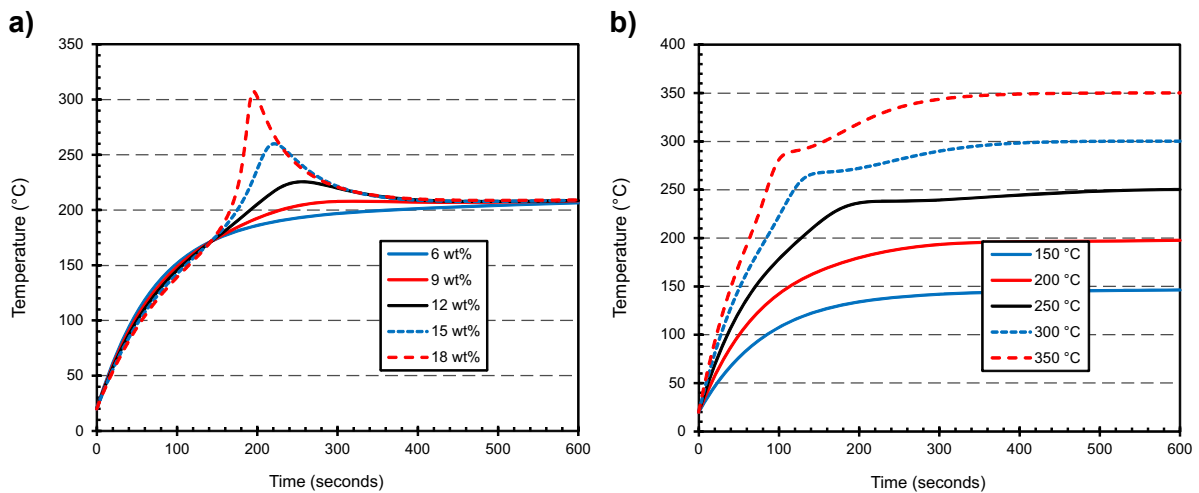


Figure 4.8: Predicted bean temperature a) at varying initial moisture content (inlet air temperature constant) and b) at varying inlet air temperature (initial moisture content constant).

The slight deviation observed in the bean temperature at the higher inlet air temperatures (as presented in Figure 4.8 (b)), can also be related to the fast moisture loss rate shown in Figure 4.6 (b).

The roast profile, which is directly determined from the bean temperature as described by Equation 4.15, was calculated for the various initial moisture content and inlet air temperature and displayed by Figure 4.9. From Figure 4.9 (a), it can be seen that the peaks caused by the rapid loss of moisture in the bean temperature, are also present in the roast profile, causing an overestimated roast profile. The slight deviation present in the bean temperature for the various inlet air temperatures (as shown in Figure 4.8 (b)), have very little effect on the predicted roast profiles as displayed in Figure 4.9 (b), and it is only logical that an increased inlet air temperature will cause a more rapidly progressing roast.

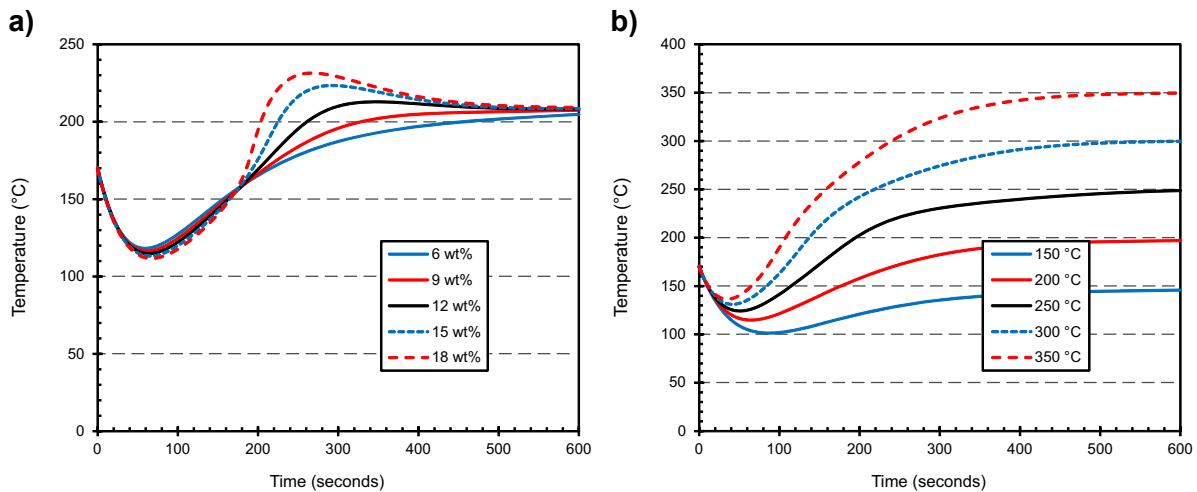


Figure 4.9: Predicted roast profile a) at varying initial moisture content (inlet air temperature constant) and b) at varying inlet air temperature (initial moisture content constant).

From this, it is concluded that the moisture loss model proposed by Schwartzberg (2002), is highly sensitive to the initial moisture content of the coffee beans and less so to the inlet air temperature. The model will start to lose its accuracy as the initial moisture content exceeds 9 wt%, and although slight disturbances will be found for the higher inlet air temperatures, the model will still accurately predict the bean temperature during the roasting process for inlet air temperatures at 350 °C. Therefore it is concluded that an improvement in the moisture content prediction will improve the bean temperature prediction and thus also the predicted roast profile.

In order to investigate whether or not an improved moisture loss model will account for a better prediction of the moisture content and temperature of the bean, the moisture loss model proposed by Hernández-Díaz *et al.* (2008) is implemented instead of the one proposed by Schwartzberg (2002) during bean temperature determination. The moisture loss is determined

using Equation 4.58, where the slope was optimised through regression to represent a faster drying rate as the one used by Hernández-Díaz *et al.* (2008).

$$\frac{dX_b}{dt} = -\frac{0.032D_b}{L^2}(X_b - X_{eq}) \quad \text{Equation 4.58}$$

The bean temperature is determined with the model parameters required for simulation taken from Table 4.7. The heat capacity and thermal conductivity determined to be the best suited for modelling in Section 4.6.1 (model Sch_Cp2_λ1) are used here with the moisture loss model described by Equation 4.58 (model Sch_Cp2_λ1_HDX). Considering the above-mentioned, the bean temperature and moisture content are simulated for the given roasting conditions and the statistical fitting efficiency parameters determined for the simulated results are presented in Table 4.11.

Implementing Equation 4.58 instead of the Schwartzberg (2002) proposed moisture loss model (Equation 4.14), resulted in a slightly better agreement between the literature and simulated data as shown in Table 4.11. For both inlet air conditions, the simulated bean temperature using model Sch_Cp2_λ1_HDX had no significant improvement above that of the simulated results obtained by model Sch_Cp2_λ1. The same was found for the moisture content determination at inlet air temperature at 210 °C. There was, however, an improvement on the moisture content determination at inlet air temperature at 250 °C, where the MRE value decrease by 5 % and the coefficient of determination increased by 0.05.

Table 4.11: Statistical fitting efficiency parameters determination for predicted bean temperature and moisture content at 210 °C and 250 °C, for models Sch_Cp2_λ1_HDX and Sch_Cp2_λ1.

Model		210 °C			250 °C		
		R ²	RSME	MRE	R ²	RSME	MRE
Bean temperature	Sch_Cp2_λ1_HDX	0.981	7.64	5.53	0.978	8.88	5.84
	Sch_Cp2_λ1	0.974	8.21	5.78	0.973	9.81	6.18
Moisture content	Sch_Cp2_λ1_HDX	0.976	0.70	14.8	0.809	1.63	47.1
	Sch_Cp2_λ1	0.955	0.90	14.7	0.749	1.93	52.3

This indicates that the moisture loss model proposed by Hernández-Díaz *et al.* (2008), could predict the moisture content more accurately at higher inlet air temperatures. The bean temperature and moisture content results obtained from this model compared to the experimental results obtained by Heyd *et al.* (2007) are presented in Figure 4.10 and Figure 4.11.

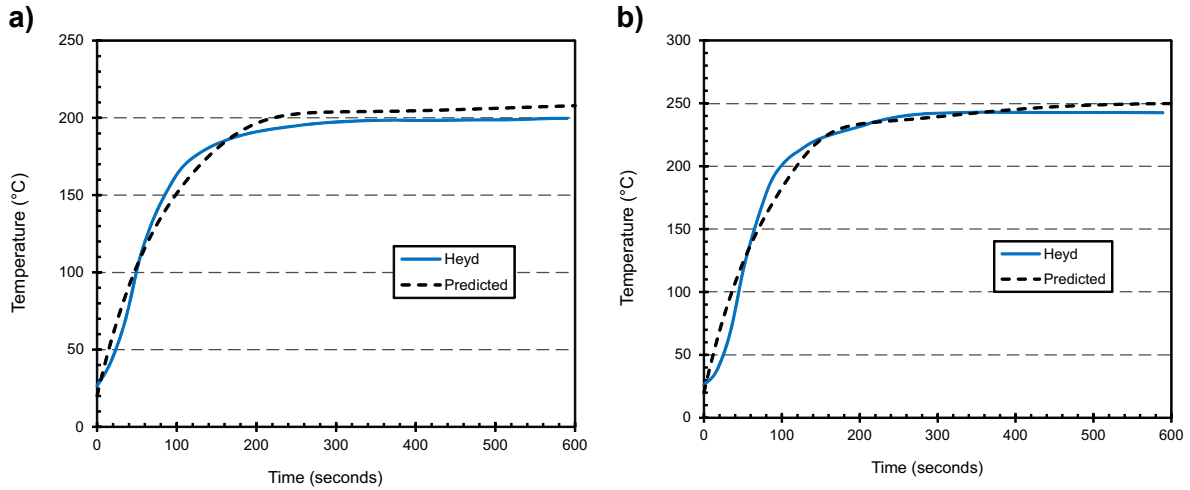


Figure 4.10: Adjusted moisture model (Sch_Cp2_λ1_HDX) to bean temperature obtained from literature data at a) 210 °C inlet air temperature and b) 250 °C inlet air temperature.

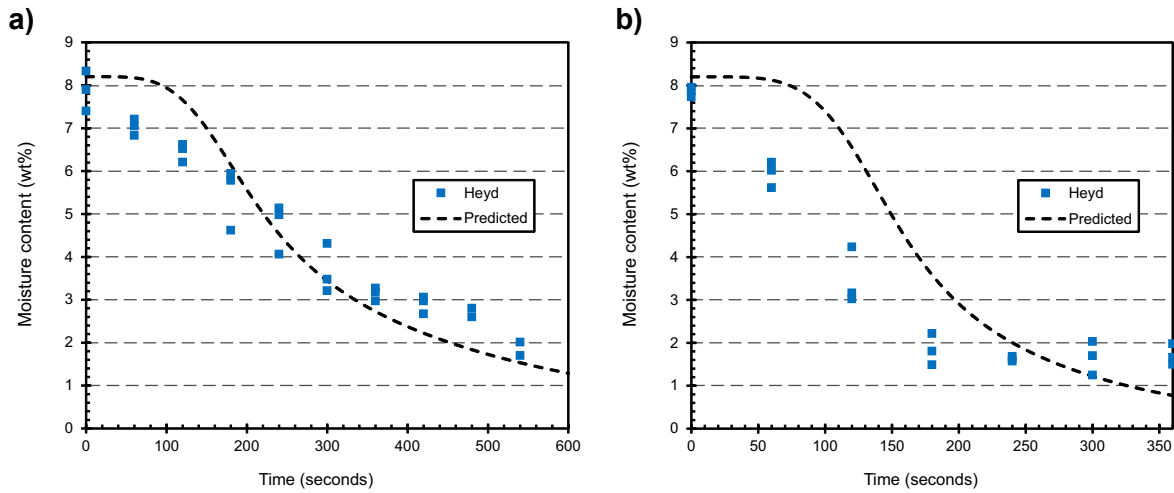


Figure 4.11: Adjusted moisture model (Sch_Cp2_λ1_HDX) to moisture content obtained from literature data at a) 210 °C inlet air temperature and b) 250 °C inlet air temperature.

The equation proposed by Hernández-Díaz *et al.* (2008) to determine the moisture content of coffee beans during roasting (Equation 4.58) was further investigated. This was done to see what effect a difference in inlet air temperature and initial moisture content will have on the accuracy of the model. Using the values presented in Table 4.7, the roasting process was first simulated for varying initial moisture content values at a constant inlet air temperature and then for varying inlet air temperatures at a constant initial moisture content.

The effect these variations in values had on the moisture content during the roasting process can be seen in Figure 4.12. In Figure 4.12 (a), the same behaviour of the moisture content can be observed in Figure 4.6 (a), however, in this case the drying rate is not as drastic and compares better to the results obtained by Schenker (2000) (shown in Figure 4.7).

The effect the inlet air temperature has on the moisture content during the roasting process is presented in Figure 4.12 (b) and depicts the same behaviour as shown in Figure 4.6 (b), where the higher the inlet air temperature, the faster the moisture will evaporate from the beans

(Burmester & Eggers, 2010). For the higher temperatures, the rate of moisture loss is fairly fast and seems almost impossible. Again, at the higher temperature, the bulk of the moisture is lost in less than 100 s. From this, it is determined that the moisture loss model proposed by Hernández-Díaz *et al.* (2008) showed a slightly better fit to literature results than that obtained by the model proposed by Schwartzberg (2002), and that it can better simulate higher initial moisture contents.

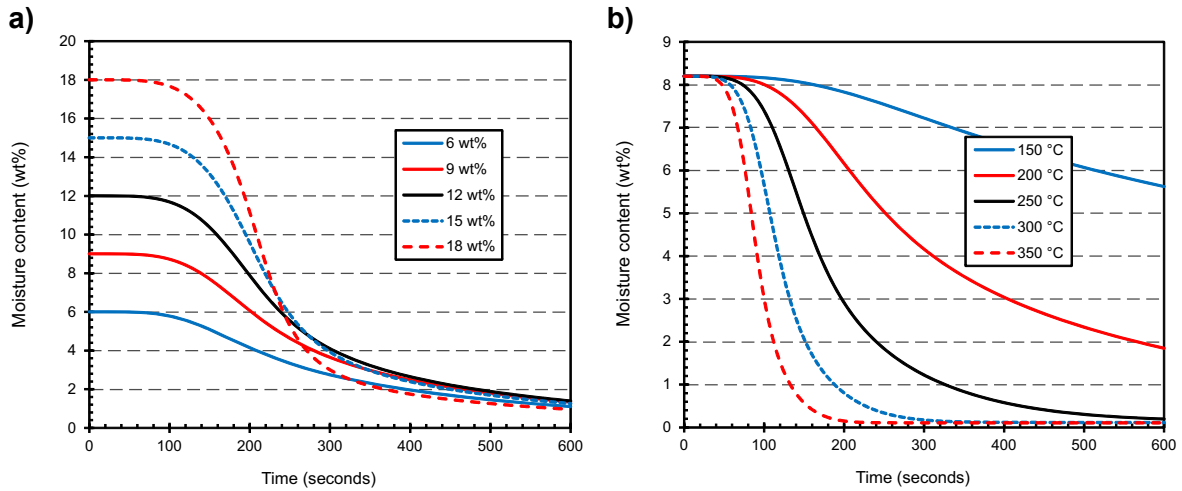


Figure 4.12: Predicted moisture content a) at varying initial moisture content (inlet air temperature constant) and b) at varying inlet air temperature (initial moisture content constant).

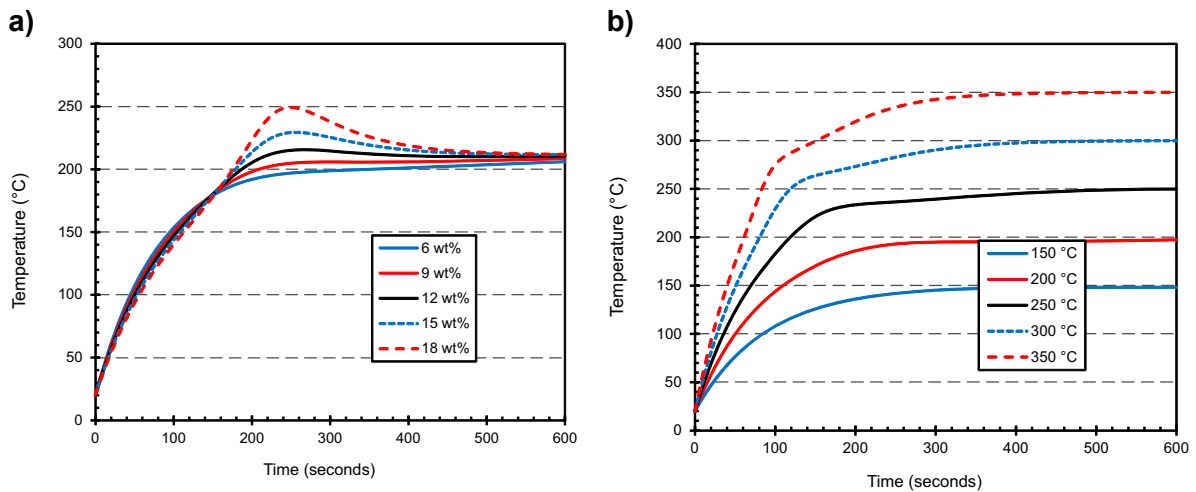


Figure 4.13: Predicted bean temperature a) at varying initial moisture content (inlet air temperature constant) and b) at varying inlet air temperature (initial moisture content constant).

The same is seen for the modelled bean temperature, where the modelled results show smaller deviations than that of the model proposed by Schwartzberg (2002), as displayed in Figure 4.13. The bean temperature overestimated in Figure 4.13 (a) is just about 50 °C, indicating that with the moisture loss model proposed by Hernández-Díaz *et al.* (2008), the bean temperature is better predicted and consequently the roast profile will also have a better prediction, as can be seen in Figure 4.14

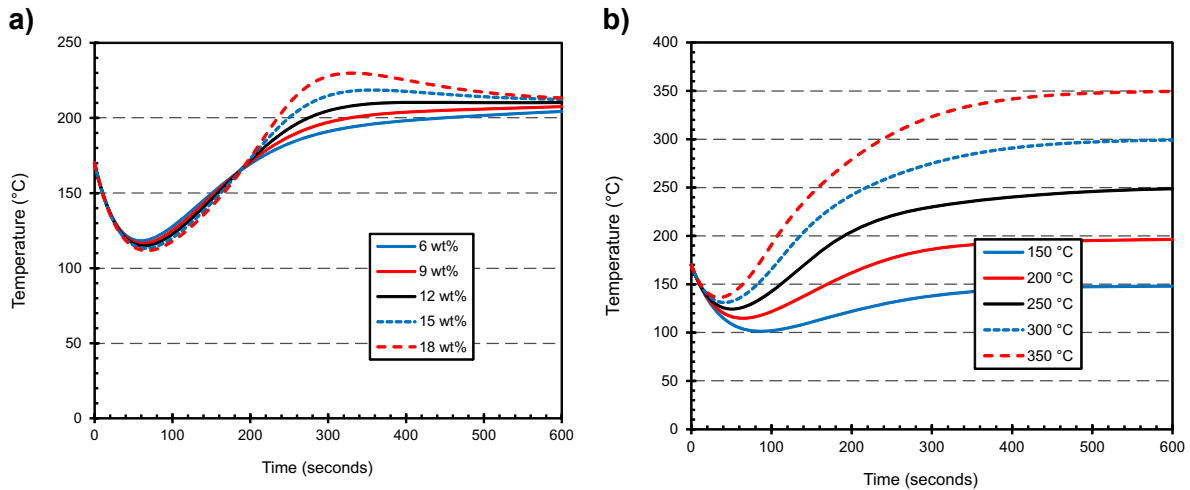


Figure 4.14: Predicted roast profile a) at varying initial moisture content (inlet air temperature constant) and b) at varying inlet air temperature (initial moisture content constant).

4.6.2 Putranto & Chen (2012)

The Putranto & Chen (2012) LREA model discussed in Section 4.1.2 is implemented as described in Section 4.5, with the model parameters required for simulation taken from Table 4.7. As discussed previously, four equations have been obtained to calculate the heat capacity of the coffee beans (Table 4.5) where only the three specified in Section 4.3.1 are further used during modelling. This model does not incorporate the thermal conductivity of the coffee beans, therefore only the different heat capacities will be considered.

In Table 4.12, the combination in which the heat capacity equations were implemented during modelling is illustrated.

Table 4.12: Combination of heat capacity of coffee beans used during modelling.

Heat capacity	Model name
(Schwartzberg, 2002)	Put_Cp1
(Putranto & Chen, 2012)	Put_Cp2
(Hernández-Díaz <i>et al.</i> , 2008)	Put_Cp3

Using the above-mentioned parameters and equations, the bean temperature and moisture content were simulated for the given roasting conditions. In Table 4.13 and Table 4.14, statistical fitting efficiency parameters are tabulated for the simulated bean temperature and moisture content respectively.

Table 4.13: Statistical fitting efficiency parameters determination for predicted bean temperature at 210 °C and 250 °C.

Model	210 °C			250 °C		
	R ²	RSME	MRE	R ²	RSME	MRE
Put_Cp1	0.972	8.4	6.16	0.963	12.2	7.84
Put_Cp2	0.986	8.6	6.14	0.982	9.1	6.01
Put_Cp3	0.980	7.8	5.57	0.977	9.1	5.88

For the simulated bean temperature at both inlet air temperatures, all three heat capacities showed good correlation to the literature data, where the highest error obtained between the simulated and literature data was 12.2 °C and all the R² values were in excess of 0.9, indicating a good relationship between the simulated and predicted data. The heat capacities proposed by Putranto & Chen (2012) and Hernández-Díaz *et al.* (2008) gave the best fit to literature data, as can be seen in Table 4.13.

Table 4.14: Statistical fitting efficiency parameters determination for predicted moisture content at 210 °C and 250 °C.

Model	210 °C			250 °C		
	R ²	RSME	MRE	R ²	RSME	MRE
Put_Cp1	0.874	3.68	106	0.499	4.94	226
Put_Cp2	0.890	3.63	104	0.522	4.85	222
Put_Cp3	0.876	3.66	105	0.498	4.90	224

Unfortunately, the simulated moisture content at both inlet air temperatures showed a very poor correlation between the simulated and literature data. The moisture loss was severely underestimated (as depicted in Figure 4.16) and the lowest error calculated between simulated and literature data were 3.63 wt%. For the inlet air temperature of 250 °C, the smallest error obtained were 4.85 wt% (taking into account that the initial moisture content is 8.2 wt%) and all the R² values were inferior to 0.6, indicating a poor relationship between simulated and literature data. The relative error for both inlet air temperatures is very high, yielding 105 % and 220 % respectively.

The bean temperature and moisture content results obtained from Put_Cp2, which had the overall best correlation to the literature data at the various roasting conditions, compared to the experimental results obtained by Heyd *et al.* (2007) are presented in Figure 4.15 and Figure 4.16.

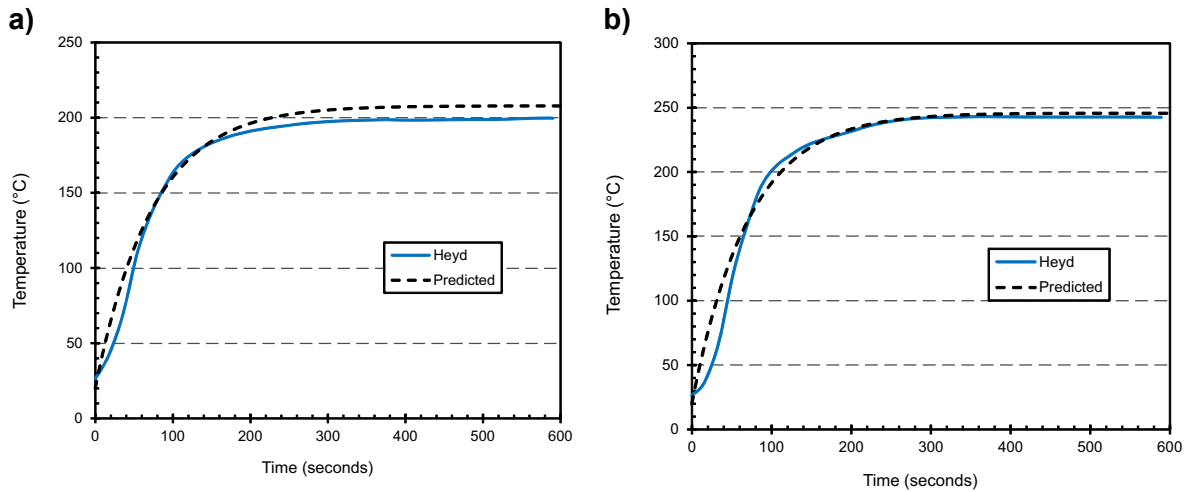


Figure 4.15: Best model fit (Put_Cp2) to bean temperature obtained from literature data at a) 210 °C inlet air temperature and b) 250 °C inlet air temperature.

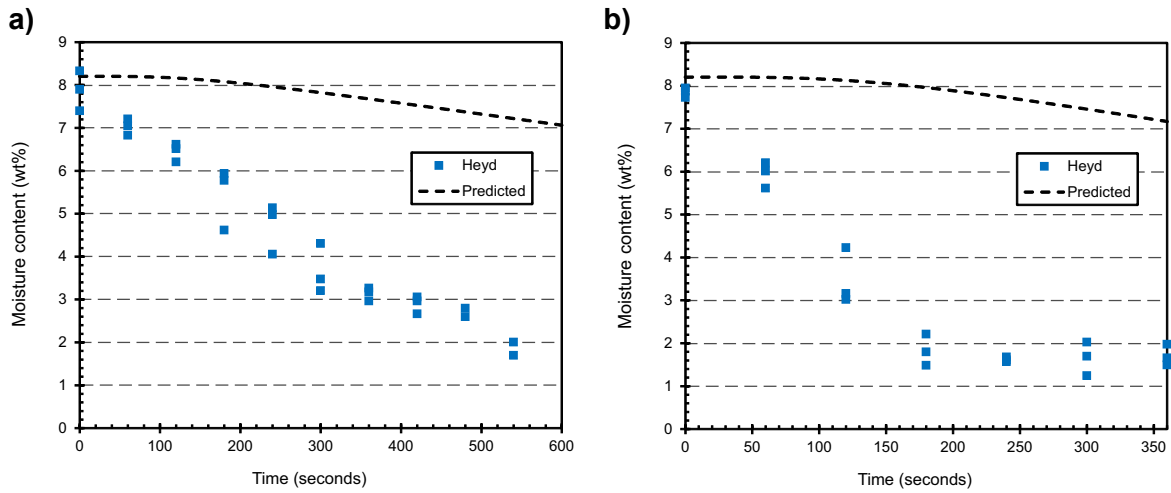


Figure 4.16: Best model fit (Put_Cp2) to moisture content obtained from literature data at a) 210 °C inlet air temperature and b) 250 °C inlet air temperature.

After further investigation, it was determined that the calculated mass transfer coefficient had a significant influence on the simulated moisture loss. In Table 4.15, the mass transfer coefficient values calculated from Equation 4.51 are presented. As stated in Section 4.2, the mass transfer coefficient has been reported to range between 3.3×10^{-4} m/s and 4.8×10^{-5} m/s (Ramirez-Martinez *et al.*, 2010). The calculated mass transfer coefficients fall within this range, however for this model it seems to be too small, resulting in a lower moisture loss rate.

Table 4.15: Calculated mass transfer coefficients (m/s).

Model name	210 °C	250 °C
Put_Cp1	2.15×10^{-5}	2.37×10^{-5}
Put_Cp2	2.17×10^{-5}	2.43×10^{-5}
Put_Cp3	2.16×10^{-5}	2.40×10^{-5}

Therefore, to obtain a better moisture loss prediction, the mass transfer coefficient was optimised with regression and a value of 2×10^{-4} m/s were used.

Using the above-mentioned adjustment and LREA model equations, the bean temperature and moisture content were modelled again for the given roasting conditions. In Table 4.16 and Table 4.17, the statistical fitting efficiency parameters were calculated for the simulated bean temperature and moisture content respectively.

Table 4.16: Statistical fitting efficiency parameters determination for predicted bean temperature at 210 °C and 250 °C, with adjusted mass transfer coefficient.

Model	210 °C			250 °C		
	R ²	RSME	MRE	R ²	RSME	MRE
Put_Cp1	0.978	8.0	5.80	0.970	17.8	11.3
Put_Cp2	0.988	5.7	4.18	0.981	14.2	9.35
Put_Cp3	0.987	6.2	4.40	0.982	14.8	9.33

With the adjusted mass transfer coefficient, the simulated results for the inlet air temperature of 210 °C, had a slightly better correlation with literature data. The highest error obtained between the simulated and literature results were 8.6 °C for the calculated mass transfer coefficient, and for the adjusted mass transfer coefficient it is 8 °C (as can be seen in Table 4.16). For the inlet air temperature of 250 °C, there was a slight increase in errors (12.2 to 17.8 °C) and therefore a weaker correlation between the simulated and literature data. However, the overall fit of the predicted results compared to the literature results is still very good.

From Table 4.17, it can be seen that the adjusted mass transfer coefficient significantly improved the modelled results compared to the literature results. For the inlet air temperature of 210 °C, the relative error decreased from about 100 to about 25 %. Where the relative error for the air temperature at 250 °C, decreased from 225 to 115 %. From Table 4.16 and Table 4.17, it was determined that the modelling with the heat capacity proposed by Putranto & Chen (2012) had the best fit of the predicted data to the literature results.

Table 4.17: Statistical fitting efficiency parameters determination for predicted moisture content at 210 °C and 250 °C, with adjusted mass transfer coefficient.

Model	210 °C			250 °C		
	R ²	RSME	MRE	R ²	RSME	MRE
Put_Cp1	0.915	1.25	24.4	0.567	2.99	115
Put_Cp2	0.928	1.09	21.5	0.599	2.70	95.7
Put_Cp3	0.916	1.21	22.6	0.570	2.89	107

The bean temperature and moisture content results obtained from Put_Cp2 and the adjusted mass transfer coefficient, which had the better correlation to the literature data at the various roasting conditions, compared to the experimental results obtained by Heyd *et al.* (2007) are presented in Figure 4.17 and Figure 4.18.

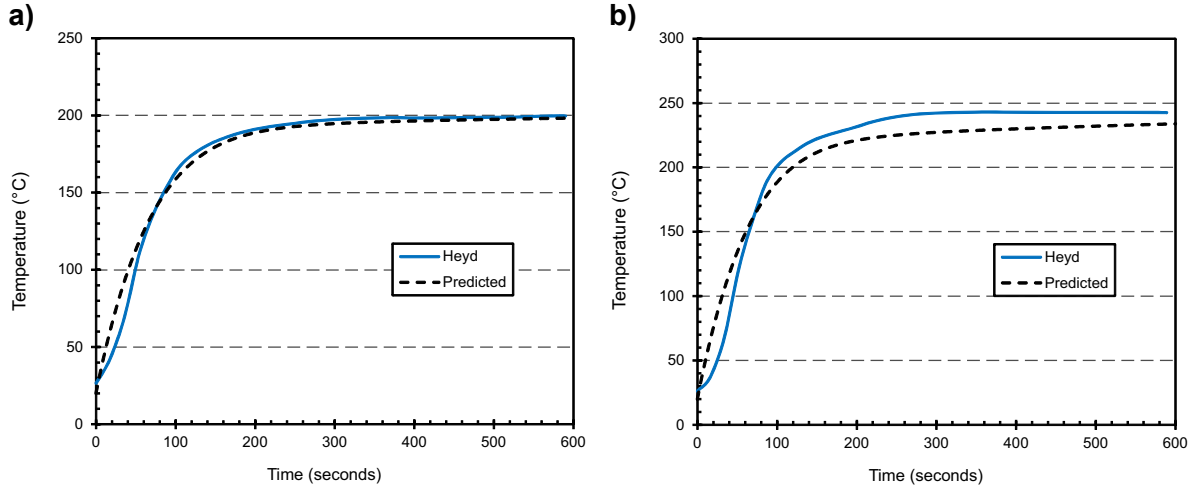


Figure 4.17: Best model fit (Put_Cp2) to bean temperature obtained from literature data at a) 210 °C inlet air temperature and b) 250 °C inlet air temperature

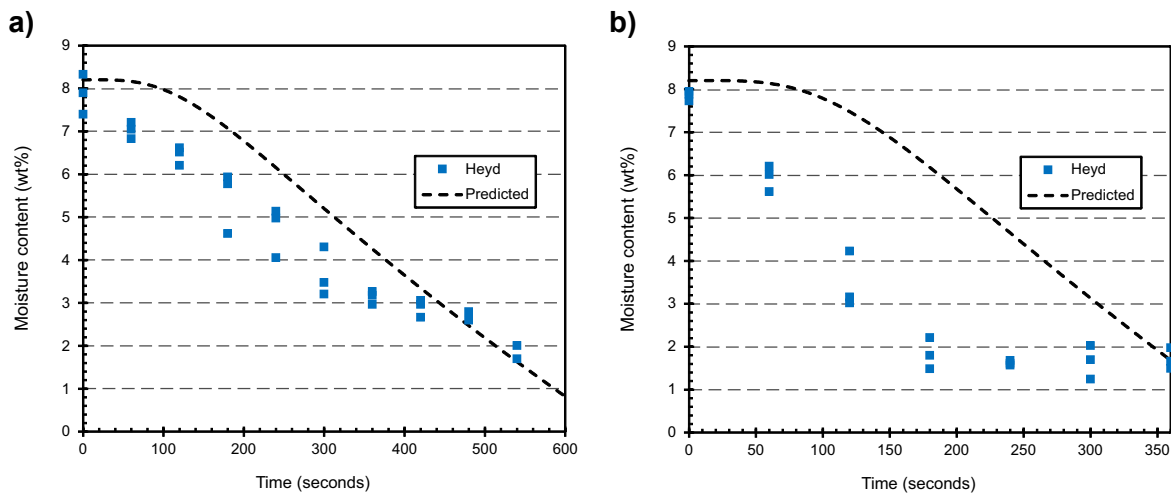


Figure 4.18: Best model fit (Put_Cp2) to moisture content obtained from literature data at a) 210 °C inlet air temperature and b) 250 °C inlet air temperature

The same procedure followed executed above, was followed here to investigate the range in which the moisture content model will still function. This was done to see what effect a difference in inlet air temperature and initial moisture content will have on the accuracy of the model. Using the values presented in Table 4.7, the roasting process was first simulated for varying initial moisture content values at a constant inlet air temperature and then for varying inlet air temperatures at a constant initial moisture content.

The effect these variations in values had on the moisture content during the roasting process can be seen in Figure 4.19. As seen in Figure 4.19, the moisture loss model proposed by Putranto & Chen (2012) had a significantly different behaviour than those of Schwartzberg

(2002) and Hernández-Díaz *et al.* (2008) at constant initial bean temperature and moisture content. The modelled results from Putranto & Chen (2012) shows a more realistic response to increased moisture content and bean temperature.

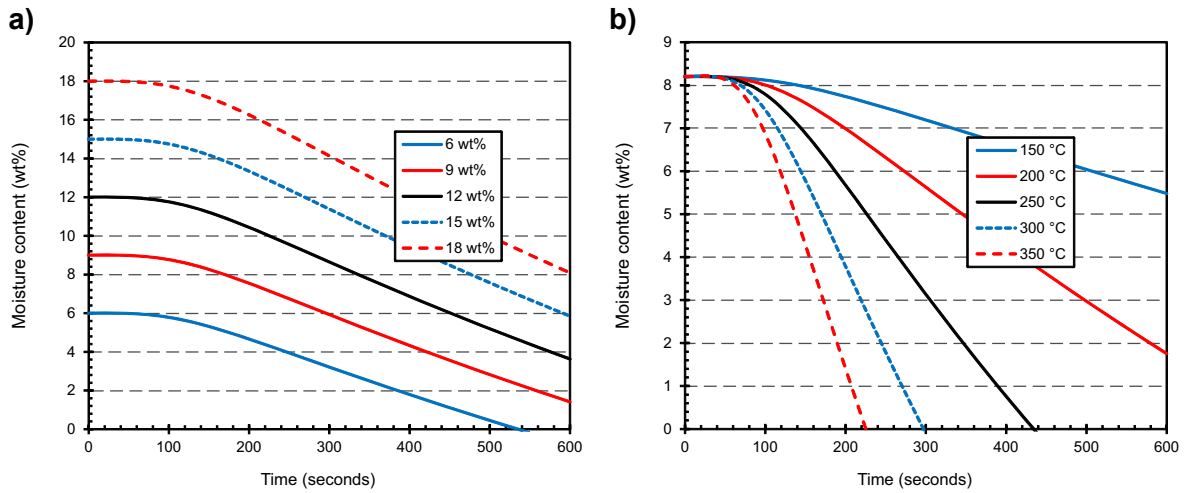


Figure 4.19: Predicted moisture content a) at varying initial moisture content (inlet air temperature constant) and b) at varying inlet air temperature (initial moisture content constant).

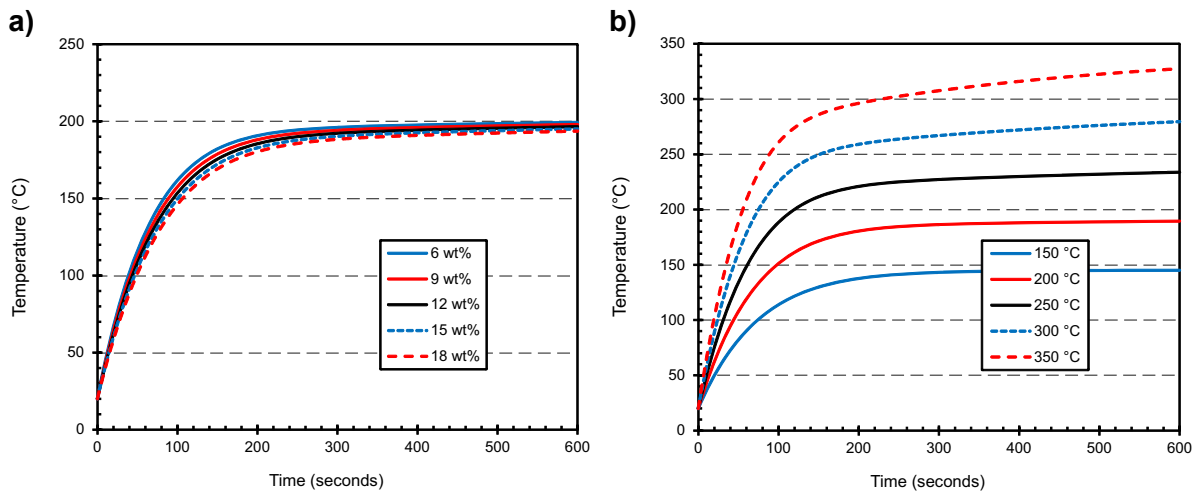


Figure 4.20: Predicted bean temperature a) at varying initial moisture content (inlet air temperature constant) and b) at varying inlet air temperature (initial moisture content constant).

From the modelled bean temperature and roast profiles, depicted in Figure 4.20 and Figure 4.21 respectively, no disturbances or peaks can be observed for the variation in conditions. These models give a more accurate response to the variation in initial moisture content and bean temperature.

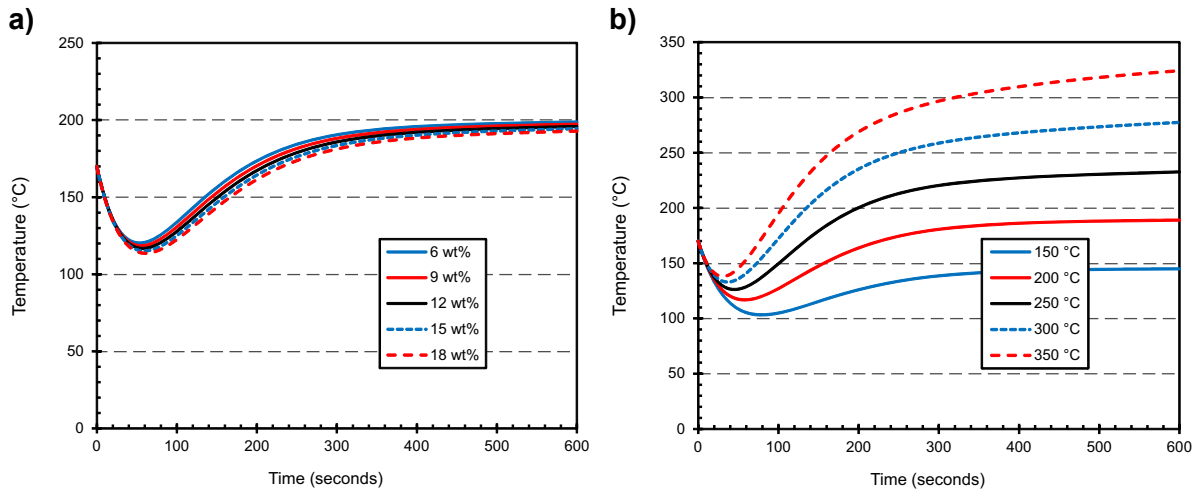


Figure 4.21: Predicted roast profile for a) at varying initial moisture content (inlet air temperature constant) and b) at varying inlet air temperature (initial moisture content constant).

4.6.3 Finite volume heat conduction in a sphere

The heat conduction in a sphere model discussed in Section 4.1.3 is solved as described in Section 4.5, using model parameters depicted in Table 4.18. The heat conduction in a sphere model is set up to consider one bean during roasting, therefore the modelled results are compared to literature results obtained for the roasting of an individual bean.

Fabbri *et al.* (2011) conducted roasting experiments with single green coffee beans roasted at 200 °C for 10 minutes. The initial values and model parameters needed to model the roasting process at these conditions are presented in Table 4.18, and the simulated bean temperature and moisture content are compared to experimental results obtained by Fabbri *et al.* (2011), for roasting at an inlet air temperature of 200 °C.

Table 4.18: Literature values used for model verification, adapted from (Fabbri *et al.*, 2011; Hernández *et al.*, 2007).

Parameter	Value
A_b	$1.4 \times 10^{-4} \text{ m}^2$
d_b	$6.6 \times 10^{-3} \text{ m}$
$m_{b(d.b)}$	$1.75 \times 10^{-4} \text{ kg d.b.}$
$T_{b,i}$	25 °C
$T_{g,i}$	200 °C
t	600 s
v_g	0.02 m/s
$X_{b,i}$	0.152 kg/kg d.b.

The heat conduction in a sphere model only considered the bean temperature during the roasting process, therefore, to simulate the moisture content during roasting the bean temperature has to be combined with a moisture loss model. For this the moisture loss models proposed by Schwartzberg (2002) and Hernández-Díaz *et al.* (2008) are considered.

In Table 4.19, the combinations of equations for heat capacity and thermal conductivity of coffee beans are shown. This modelling is repeated for both moisture loss models.

Table 4.19: Combination of heat capacity and thermal conductivity of coffee beans used during modelling.

Heat capacity	Thermal conductivity	Model name
(Schwartzberg, 2002)	(Hernandez, 2002)	Peb_Cp1_λ1
	(Hernández-Díaz <i>et al.</i> , 2008)	Peb_Cp1_λ2
(Putranto & Chen, 2012)	(Hernandez, 2002)	Peb_Cp2_λ1
	(Hernández-Díaz <i>et al.</i> , 2008)	Peb_Cp2_λ2
(Hernández-Díaz <i>et al.</i> , 2008)	(Hernandez, 2002)	Peb_Cp3_λ1
	(Hernández-Díaz <i>et al.</i> , 2008)	Peb_Cp3_λ2

Using the above-mentioned parameters and equations, the bean temperature and moisture content were modelled for the given roasting conditions. In Table 4.20 and Table 4.21, statistical fitting efficiency parameters are tabulated for the modelled bean temperature and moisture content respectively.

The results obtained from the modelled bean temperature (as seen in Table 4.20) for both moisture loss models, and the proposed heat capacity and thermal conductivity, showed an average fit to the literature data. As can be seen from Figure 4.22, the model initially predicted the bean temperature according to the literature data, however just as the bean temperature reached 100 °C, the simulated results deviated from the literature results, showing a brief temperature spike before steadily increasing in temperature. Both models underestimate the bean temperature as the temperature increases and at the end there is about a 30 °C difference between the simulated and the literature data.

From Table 4.20, it can be seen that the bean temperature combined with the moisture loss model proposed by Schwartzberg (2002) had a slightly better fit to the literature data (with the highest error between simulated and literature results being 25.6 °C compared to the 31.8 °C obtained by the other model).

Table 4.20: Statistical fitting efficiency parameters determination for predicted bean temperature with the moisture loss model of Hernández-Díaz *et al.* (2008) and Schwartzberg (2002).

Model	(Hernández-Díaz <i>et al.</i> , 2008)			(Schwartzberg, 2002)		
	R ²	RSME	MRE	R ²	RSME	MRE
Peb_Cp1_λ1	0.934	31.8	18.6	0.886	25.6	17.6
Peb_Cp1_λ2	0.970	30.5	14.7	0.963	21.8	10.4
Peb_Cp2_λ1	0.900	31.8	20.4	0.873	25.8	17.6
Peb_Cp2_λ2	0.964	30.0	14.4	0.953	21.7	10.8
Peb_Cp3_λ1	0.928	31.4	18.6	0.912	24.2	15.2
Peb_Cp3_λ2	0.979	30.8	16.2	0.969	22.1	11.6

The moisture content results show the exact opposite, where the moisture loss model proposed by Hernández-Díaz *et al.* (2008) had a considerably better fit than that of Schwartzberg (2002) (with the highest error between simulated and literature results being 0.415 wt% compared to the 3.02 wt% obtained by the other model) and as can be seen from Figure 4.23.

Table 4.21: Statistical fitting efficiency parameters determination for predicted moisture content with the moisture loss model of Hernández-Díaz *et al.* (2008) and Schwartzberg (2002).

Model	(Hernández-Díaz <i>et al.</i> , 2008)			(Schwartzberg, 2002)		
	R ²	RSME	MRE	R ²	RSME	MRE
Peb_Cp1_λ1	0.996	0.415	7.49	0.995	3.02	55.9
Peb_Cp1_λ2	0.997	0.375	6.50	0.994	2.99	55.2
Peb_Cp2_λ1	0.995	0.400	5.64	0.995	2.95	54.6
Peb_Cp2_λ2	0.996	0.358	5.52	0.995	2.88	53.4
Peb_Cp3_λ1	0.996	0.380	6.40	0.994	3.05	56.4
Peb_Cp3_λ2	0.997	0.368	6.49	0.993	3.01	55.7

The bean temperature and moisture content results obtained from the heat conduction in a sphere model with the best overall fit (Peb_Cp2_λ2), which had the better correlation to the literature data at the various roasting conditions, compared to the experimental results obtained by Fabbri *et al.* (2011) are presented in Figure 4.22 and Figure 4.23. However, since the roast profile is determined from the bean temperature, it is concluded that the finite volume heat conduction in a sphere model will underestimate the roast profile just as it underestimated the bean temperature, and therefore it will not be sufficient to predict the roasting process.

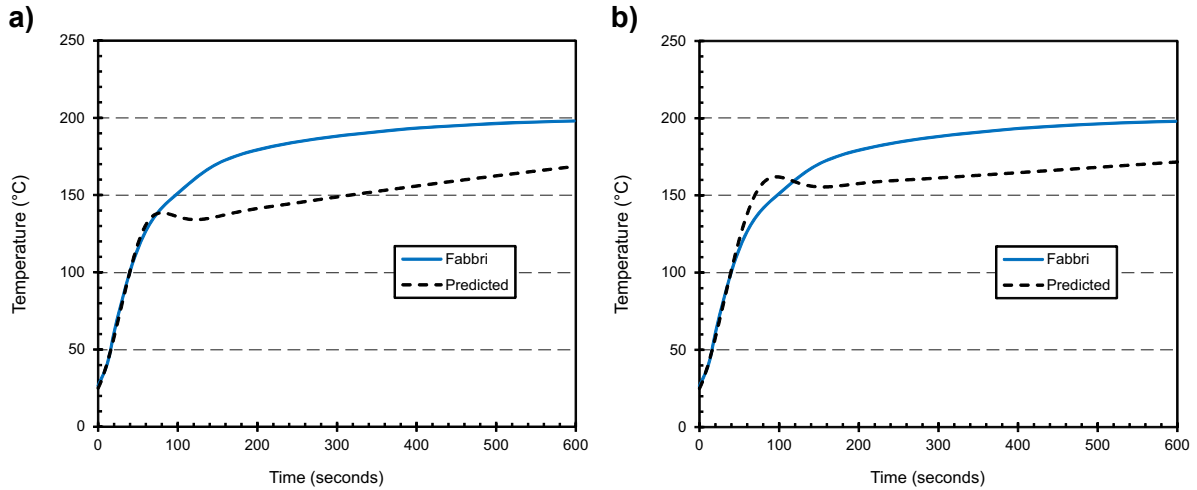


Figure 4.22: Best model fit (Peb_Cp2_λ2) to bean temperature obtained from literature data with the moisture loss model of (a) Hernández-Díaz *et al.* (2008) and (b) Schwartzberg (2002).

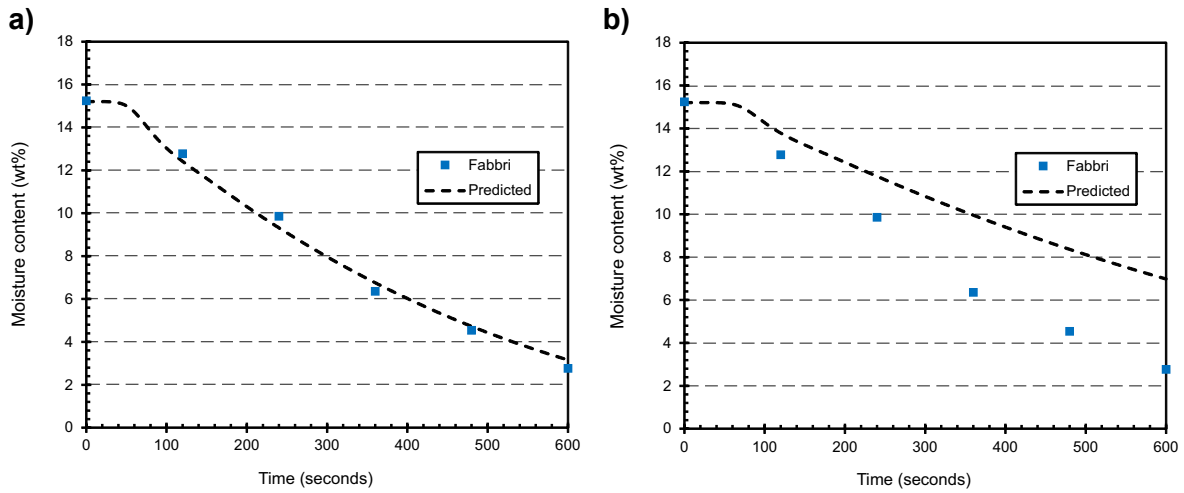


Figure 4.23: Best model fit (Peb_Cp2_λ2) to moisture content obtained from literature data with the moisture loss model of (a) Hernández-Díaz *et al.* (2008) and (b) Schwartzberg (2002).

4.7 Conclusion

From the comparative results between the derived models and models from, it was decided that the models listed in Table 4.22 will be used further investigated. This is done to determine their capability in predicting the roasting process through modelling of the bean temperature and the moisture content at the specified roasting conditions, and from the obtained results simulating the roast profile.

The heat capacity and thermal conductivity formulas that will be used for modelling are the heat capacity proposed by (Putranto & Chen, 2012) and the thermal conductivity proposed by Hernandez (2002). The roast profile for all three considered models will be calculated using the modelled bean temperature and Equation 4.15.

Table 4.22: Models considered for roast profile predictions.

Bean temperature	Moisture content	Model name
(Schwartzberg, 2002) Equation 4.6	(Schwartzberg, 2002) Equation 4.14	Sch_TX
(Schwartzberg, 2002) Equation 4.6	(Hernández-Díaz <i>et al.</i> , 2008) Equation 4.58	Sch_T_HDX
(Putranto & Chen, 2012) Equation 4.16	(Putranto & Chen, 2012) Equation 4.21	Put_TX

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CHAPTER 5 – Results and discussion

Overview

Chapter 5 focusses on the results obtained from the roasting experiments in comparison with results obtained from the heat and mass transfer models. The main focus here is to validate the roast profile determined from the heat and mass transfer model, with the experimental data obtained. This is done by first comparing the modelled moisture content with the moisture content acquired from the experiments conducted, and subsequently comparing the roast profiles obtained during roasting with modelled roast profiles. The degree of roast is also estimated from the experimental results obtained from the final roasted beans and associated with the roast profile, so that a degree of roast prediction can be made from typical roast profile data.

"I have measured out my life with coffee spoons." – T.S. Eliot

5.1 Roasting for ten minutes

5.1.1 Roasting process experimental results

Batches of 4 kg raw green coffee beans were roasted at a starting roast temperature of 170 to 240 °C for 10 minutes. In Figure 5.1, the average roast profile (determined from 3 repeated roasts) of roasts starting from 170 °C, 200 °C and 240 °C are presented. As discussed in Section 2.2.4, the roast profile illustrates the temperature determined from a thermocouple inserted into the continuously agitated bean batch. The start temperature of the roast profile is the temperature of the environment around the thermocouple just before the beans are released into the rotating drum. The immediate drop in temperature (as observed from Figure 5.1 between 0 and 100 seconds during the roasting process) is just the interaction between the bean batch entering the drum at room temperature and the surrounding environment at the elevated temperature (Rao, 2014). The roasting profiles, moisture content determination during the roasting process and the determined roasting properties for all the conducted roasts can be found in Appendix G.

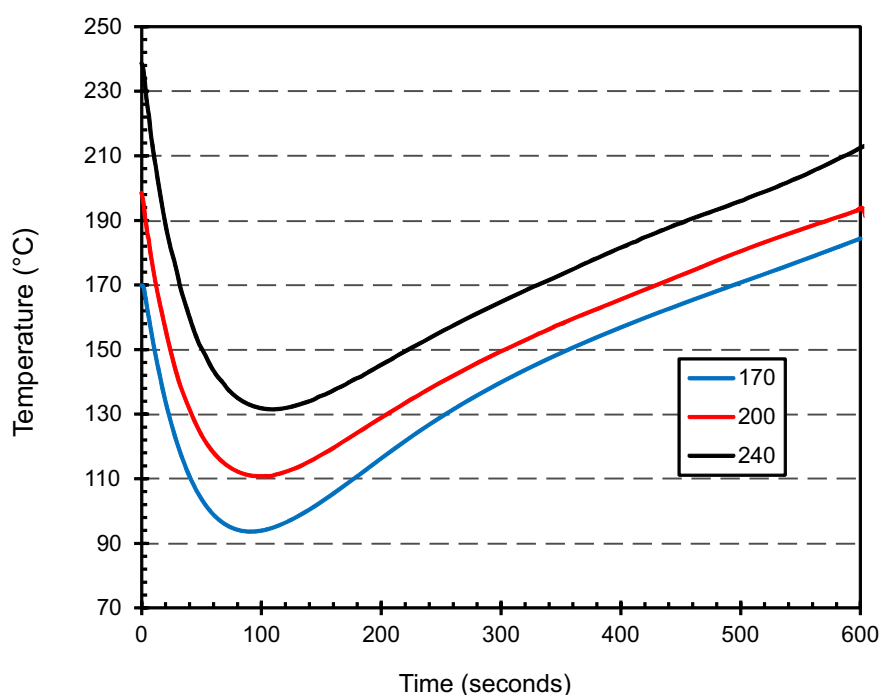


Figure 5.1: Average roast profiles of coffee roasted for 10 minutes at various temperatures.

In Figure 5.2, the average moisture content determined during the roasting process for roasts starting at respectively 170 °C, 200 °C and 240 °C is shown. As seen in Figure 5.2, the moisture content of the coffee beans decreased from 9.1 to about 1 wt%, which is similar to results obtained by Budryn *et al.* (2012); Franca *et al.* (2005) and Schenker *et al.* (2002). As the roast start temperature increased the final moisture content for the roasts at the same roasting time, decreased. From Figure 5.1 and Figure 5.2, it can be observed that the same

final temperature and moisture content can be obtained from different starting temperatures and varied roasting times (for example it can be forecasted to take approximately 600 seconds to reach an end temperature of 185 °C starting at 170 °C, but only 400 seconds to reach that end temperature when starting at 240 °C). These roasting procedures are referred to as High temperature short time (HTST) and Low temperature long time (LTLT) process conditions (Baggenstoss *et al.*, 2008; Schenker *et al.*, 2002). Artisan roasters implement these procedures according to their personal experience and taste.

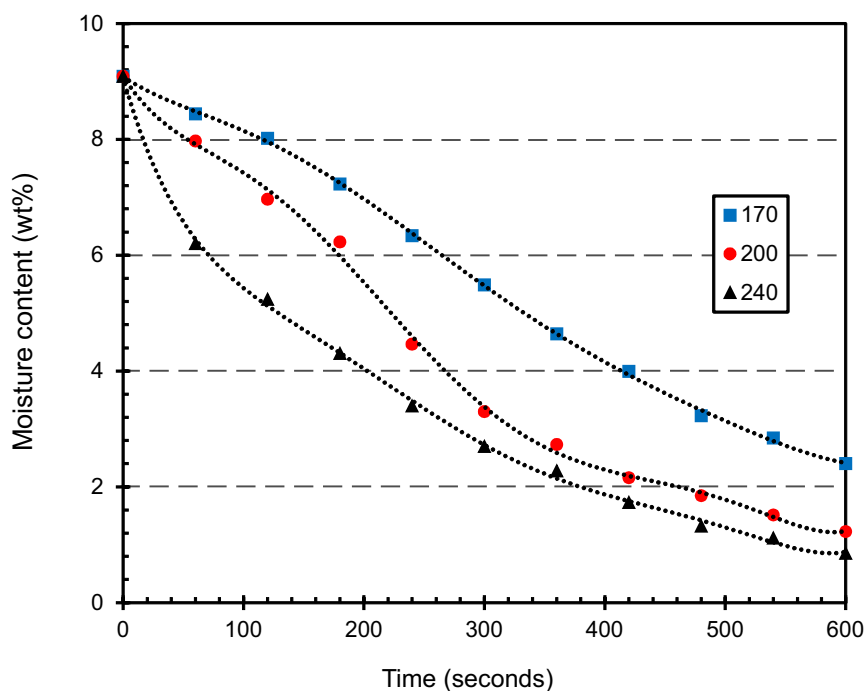


Figure 5.2: Average moisture content, during a 10 minute roasting process, of coffee for various temperatures.

The various degree of roast parameters was determined as described in Section 3.3.8 and are tabulated in Table 5.1. Along with these parameters (roast loss - RL - and final moisture content), the roast progression in terms of the occurrence of the first and second crack is also reported. Using the values and information obtained from literature (as described in Section 2.2.5) the degree of roast for every roast start temperature are determined.

The slight increase in final moisture content for the 210 °C roast, can be attributed to the formation of water during the exothermic pyrolysis reaction that occur at higher temperatures and is usually observed between the first and second crack during the roasting process (Budryn *et al.*, 2012; Wang & Lim, 2012).

As can be seen from Table 5.1, as the start temperature increases, the determined degree of roast changes from light to dark, indicating that a 600 second roast starting from 170 °C will deliver a light roast, whereas for the same length of time a roast starting at 240 °C will result in a dark roast.

For the 170 °C roast, the first crack is barely reached before the beans were extracted from the roasting drum, while for the 200 °C roast the first crack had almost ended when the roast was stopped. The 240 °C roast, on the other hand, has already reached the start of the second crack when the beans were removed from the roasting drum.

Therefore, as can be seen from Table 5.1, the roasts starting from 170 to 190 °C are classified as light roasts, while the 200 and 210 °C roasts are classified as medium roasts, and finally the 220 to 240 °C roasts are classified as dark roasts. Anything roasted beyond these will result in a very dark/burnt roast.

The end of roast temperature, which is the measured batch temperature just before the beans are removed from the roasting drum, were also noted in Table 5.1. It was observed that for the light classified roasts, the end of roast temperature barely exceeded 190 °C, while for the medium roasts the end of roast temperature ranged between 190 °C and 200 °C. The darker roasts produced end of roast temperatures exceeding 200 °C.

Table 5.1: Average roasting properties determined for the various roast start temperatures.

Roast start temp (°C)	RL (%)	Final moisture content (wt%)	Roast end temp* (°C)	Roast progression	Roast degree
170	13.1	2.40	184	Just as first crack is starting	Light
180	13.8	1.94	183	Just as first crack is starting	Light
190	14.9	1.51	191	Just as first crack is ending	Light
200	15.2	1.23	194	Just as first crack is ending	Medium
210	15.0	1.36	195	Just after first crack	Medium
220	16.1	0.86	202	Just as second crack is starting	Dark
230	15.5	1.18	202	Just as second crack is starting	Dark
240	20.1	0.85	213	During second crack	Dark

*temp is for temperature

Yeretzian *et al.* (2012) reported similar results, although the dark roasts end of roast temperature was reported to be just below 200 °C (around 198 °C). The overall roast end temperatures reported by Gloess *et al.* (2014) for Arabica coffee beans from various origins,

corroborates these results where medium roasts were found to end between 186 °C and 196 °C and the dark roasts resulted in end of roast temperatures higher than 198 °C. Using the end of roast temperature as a means of determining the roast degree have been proposed by Schwartzberg (2002), and although there may exist some overlapping between the determined end of roast temperature for the different roast degrees, this method may serve as a rudimentary roast degree prediction method based solely on the roast profile progression.

The temperatures at which first and second crack was first observed, including when the first crack ended, as well as the time into the roasting process these occurred, are presented in Table 5.2. From Table 5.2, it can be observed that regardless of the time it took to reach it, the first crack for all roast profiles started at about 175 °C, which is consistent with values reported by Gloess *et al.* (2014), and ended when the roast reached about 190 °C. The second crack started just as the bean batch reached 200 °C. This phenomenon was also described by Gloess *et al.* (2014). The temperatures reported for the start and end of first and second crack corresponds to those reported for the end of roast temperatures, further indicating the use of roast profile progression as a means of predicting the degree of roast.

Table 5.2: Temperature and roasting time for when the first and second crack occurs for 10 minute roasts.

Roast start temp* (°C)	Start first crack		End first crack		Start second crack	
	Temp (°C)	Time (s)	Temp (°C)	Time (s)	Temp (°C)	Time (s)
170	179	561	-	-	-	-
180	175	544	-	-	-	-
190	175	485	189	580	-	-
200	175	470	190	583	-	-
210	177	454	188	569	-	-
220	177	415	193	537	201	570
230	181	415	190	535	200	568
240	177	367	197	490	201	524

*temp is for temperature

5.1.2 Roasting and moisture content model validation

Modelling of the roasting process was conducted with the models proposed in Table 4.22 from Section 4.7. Henceforth these models will be referred to as Sch_TX, Sch_T_HDX and Put_TX (for an explanation of the details of these models, consult Table 4.22).

In order to accurately model the experimental roast conducted, several roasting conditions and parameters need to be determined. In Table 5.3, the roasting conditions and parameters for the various experimental roasts, determined as described in Chapter 3, are listed.

The relative humidity of the roasting air was determined with a thermohygrometer. From measured relative humidity at room temperature and also at 180 °C, it was extrapolated that for the various inlet air temperatures the relative humidity would not exceed 0.1 %. This value is confirmed by Hernández *et al.* (2007). It was also found that the Put_TX model is insensitive to small changes in this value (as shown in Appendix F).

Table 5.3: Roasting conditions and parameters determined for modelling.

Parameter	Value
A_b	3.75 m ² *
d_b	6.97×10^{-3} m
G_g	0.047 kg/s
$m_{b(d.b)}$	3.64 kg d.b.
$RH_{g,i}$	0.1 %
$T_{b,i}$	20 °C
$T_{g,i}$	See Appendix G
$T_{rp,i}$	170 - 240 °C (at 10 °C intervals)
t	600 s
v_g	0.6 m/s
$X_{b,i}$	0.091 kg/kg d.b.

Previous modelling, as discussed in Section 4.6, assumed a constant inlet air temperature during the entire roasting process. However, due to the nature of the rotating drum roaster, the inlet air temperature have a sudden drop the moment the beans are released into the drum.

Preliminary modelling was done to see what effect this change in inlet air temperature will have on the predicted roast profile compared to assuming a constant inlet air temperature, which is shown in Figure 5.3. As can be seen from Figure 5.3, when a constant inlet air temperature is used, the predicted roast profile will show a noteworthy overestimation compared to the predicted roast profile when the change in inlet air temperature is accounted for. Therefore the average inlet air temperature measured over the entire roast for every start of roast temperature was used during the modelling (which can be seen in Appendix G).

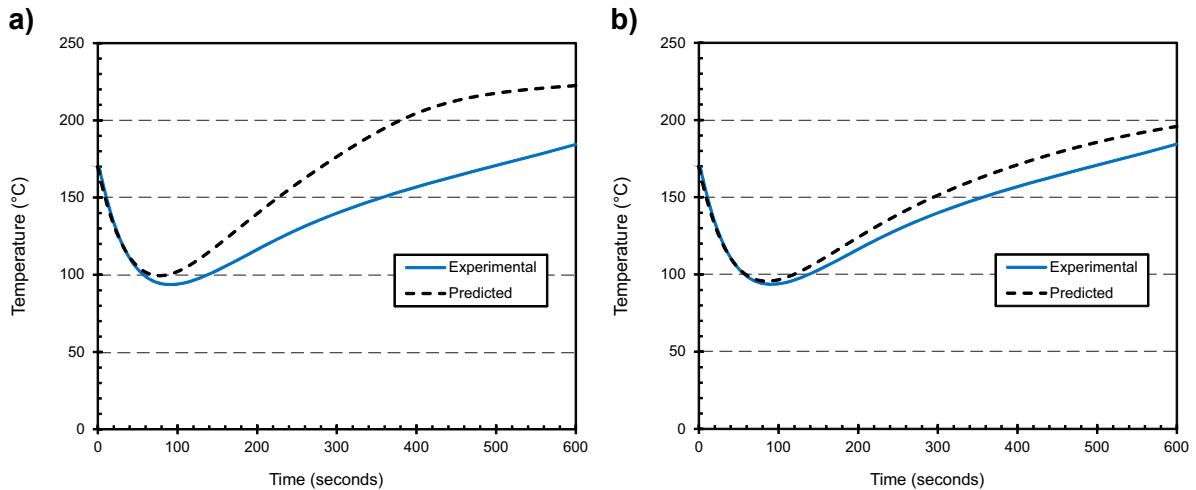


Figure 5.3: Roast profile prediction with a) assuming constant inlet air temperature and b) accounting for the change in inlet air temperature during the roasting process.

Initial modelling with the Put_TX model gave a substantial overestimation of the bean temperature and consequently the roast profile, as can be seen in Figure 5.4. It was concluded that the calculated surface area used during modelling, was too great for the proposed model, which resulted in a higher heat transfer rate taking place and therefore heating the beans much faster than in reality.

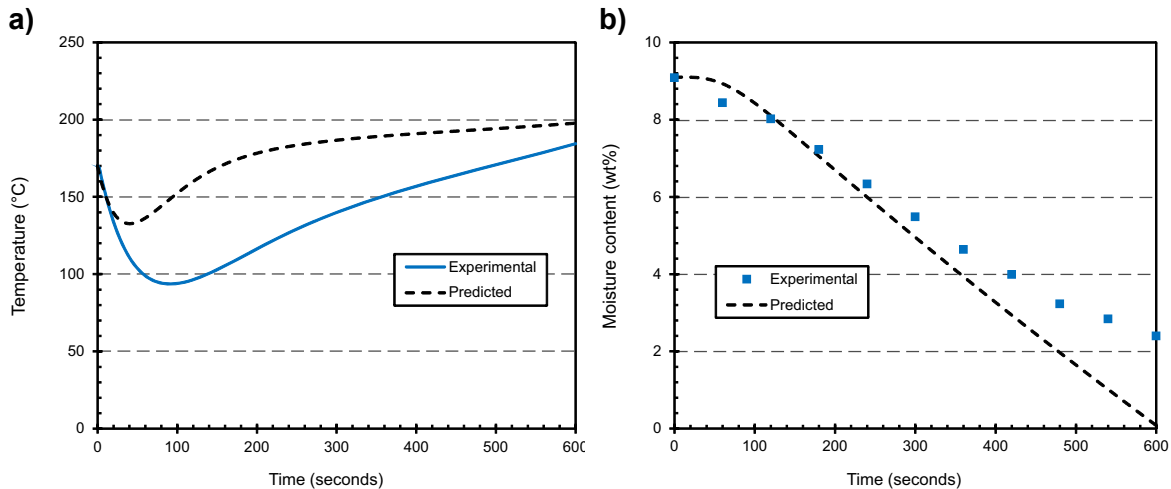


Figure 5.4: Preliminary modelling of a) the roast profile and b) the moisture content, with the Put_TX model for a start roast temperature of 170 °C.

These higher bean temperatures contributed to the faster modelled moisture loss, to such a degree that for the higher roasting temperatures, negative moisture contents were predicted (as can be seen in Appendix H). Therefore, to further evaluate the model an adjusted surface area value was determined, with regression, to better fit experimental results. A surface area of 0.9 m² was used instead of the calculated value stated in Table 5.3 (along with an adjusted mass transfer coefficient, as described in Section 4.6.2, to ensure a better moisture content prediction).

Using the above-mentioned parameters and equations, the roast profile and moisture content were modelled for the given roasting conditions, as described in Chapter 4. In Table 5.4 and Table 5.5, the statistical performance parameters (as described in Section 4.4) that were calculated for the predicted roast profile and moisture content respectively, are listed for all start of roast temperatures and the three proposed models. These values are used to determine the suitability and accuracy of the models. However, it should be noted that when using the mean relative error (MRE), a higher percentage error will be found for models that overestimate the predicted values. This is due to the fact that the MRE have a heavier penalty for positive errors than negative errors, and in fact has a limit of 100 % when values are underestimated but there is no limit when overestimation occurs (Hyndman & Koehler, 2006; Shcherbakov *et al.*, 2013). As will be seen further in this section, the moisture content models will usually overestimate the predicted values and therefore large MRE are expected for the modelled moisture content.

From the results presented in Table 5.4 and Table 5.5, it is observed that overall, all three models exhibit a fairly good fit to experimental results. All coefficients of determination, R^2 values are in excess of 0.7, and as discussed in Section 4.4, this indicates a good correlation between the predicted and experimental results, further implying that all three models can sufficiently predict the roast profile and moisture content for the given roasting conditions.

Table 5.4: Statistical fitting efficiency parameters determination for predicted roast profile of the three proposed models, for roasts continued for 10 minutes.

Roast start temp (°C)	Sch_TX			Sch_T_HDX			Put_TX		
	R^2	RSME	MRE	R^2	RSME	MRE	R^2	RSME	MRE
170	0.989	10.8	6.51	0.973	15.3	8.97	0.988	4.03	1.86
180	0.948	16.7	9.99	0.913	20.8	12.3	0.977	4.47	2.60
190	0.958	18.3	9.80	0.919	15.1	8.26	0.970	6.57	3.44
200	0.941	17.3	9.23	0.905	19.5	10.3	0.971	4.85	2.64
210	0.930	12.6	6.76	0.883	15.8	8.47	0.966	8.32	4.43
220	0.939	12.3	6.38	0.896	15.1	7.86	0.964	11.4	6.43
230	0.875	15.5	7.96	0.830	17.9	9.29	0.964	8.85	4.40
240	0.902	15.8	7.66	0.863	17.9	8.86	0.961	9.11	4.25

The Put_TX model, had the best fit to experimental results obtained for the roast profile, where the highest values obtained for the RSME and MRE are 11.4 °C and 6.43 % respectively (compared to Sch_TX's 18.3 °C and 9.99 %, and Sch_T_HDX's 20.8 °C and 12.3 %). However, when taking the moisture content prediction into account (as observed from results

listed in Table 5.5), the Put_TX had a greater error for the predicted moisture content (highest error of 165 %) compared to Sch_TX (highest error of 113 %) and Sch_t_HDX (highest error of 73.1 %). From Figure 5.5 to Figure 5.7, it can be seen that these high errors are due to an overestimation of the predicted moisture content. Where the Put_TX model made the highest overestimation of the predicted moisture content.

Table 5.5: Statistical fitting efficiency parameters determination for predicted moisture content of the three proposed models, for roasts continued for 10 minutes.

Roast start temp (°C)	Sch_TX			Sch_T_HDX			Put_TX		
	R ²	RSME	MRE	R ²	RSME	MRE	R ²	RSME	MRE
170	0.857	2.05	42.9	0.955	1.05	18.3	0.903	2.09	46.2
180	0.833	2.26	52.9	0.934	1.32	25.3	0.862	2.45	62.2
190	0.824	2.25	61.4	0.917	1.72	48.1	0.809	2.98	97.4
200	0.817	2.42	72.7	0.920	1.62	44.0	0.796	3.02	106
210	0.792	2.57	71.2	0.893	1.72	39.5	0.791	2.99	95.1
220	0.729	3.10	113	0.834	2.30	73.1	0.714	3.73	165
230	0.786	2.47	65.0	0.871	1.76	35.7	0.753	3.09	104
240	0.754	2.71	80.4	0.835	2.06	48.8	0.704	3.43	139

The results obtained from modelling the roasting process for a start of roast temperature of 170 °C, are shown in Figure 5.5 to Figure 5.7, where the predicted roast profile and moisture content are compared to experimental results for all three models. The results obtained for the other start of roast temperatures can be seen in Appendix H.

From Figure 5.5 (a), it can be seen that the Sch_TX model predicted a slightly overestimated roast profile and that the predicted model started to deviate at about 100 seconds into the roasting process. At the higher start of roast temperatures (210 to 240 °C), the predicted results had a slight deviation from the start of the roast where the Sch_TX model underestimated the roast profile at the turning point of the roast profile with about 10 °C. However, after about 160 seconds the predicted model showed the same overestimation as the other start of roast temperatures. The moisture content prediction, as seen in Figure 5.5 (b), made the overestimation from the start, indicating that the Sch_TX model assumes a slower drying rate than experimentally observed. The same was observed for all other start of roast temperatures.

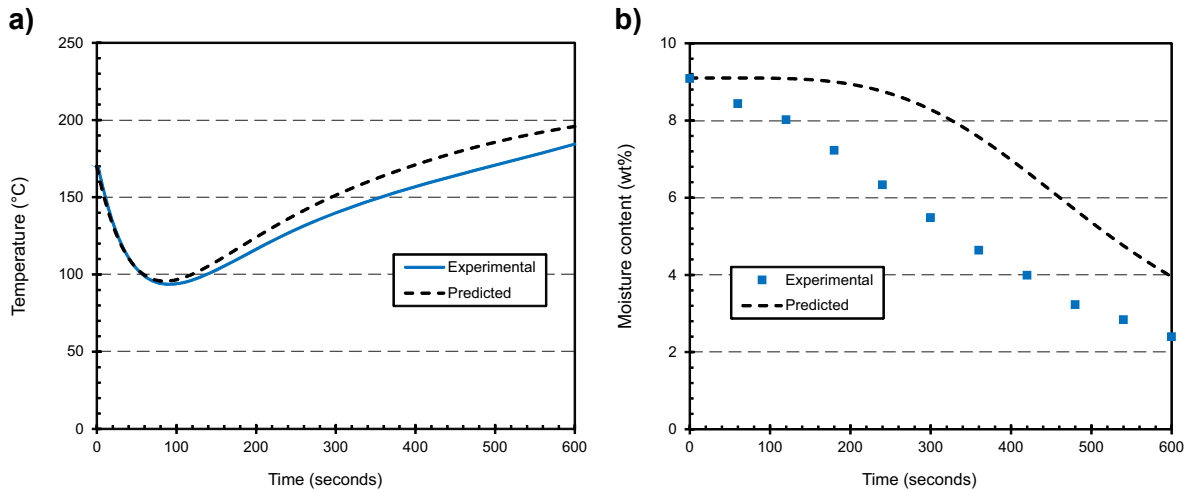


Figure 5.5: Sch_TX model fit to experimentally determined a) roast profile and b) moisture content, for a 10 minute roast at a start roast temperature of 170 °C.

From Figure 5.6 (a), it can be seen that the Sch_T_HDX model predicted the same overestimation of the roast profile than the Sch_TX model, where the predicted model started to deviate at about 100 seconds into the roasting process. However, the overestimation made by the Sch_T_HDX model were slightly higher as can be seen from the results presented in Table 5.4. At the higher start of roast temperatures (210 to 240 °C), the same behaviour is observed for the predicted roast profiles, where the predicted results underestimate the roast profile at the turning point and then after about 150 seconds the predicted model showed the same overestimation as the other start of roast temperatures. The moisture content prediction, as seen in Figure 5.6 (b), made the overestimation from the start, however compared to the Sch_TX model, the predicted drying rate is a bit faster resulting in a more accurately predicted moisture content (as shown by the results listed in Table 5.5). The same behaviour was observed for all other start of roast temperatures.

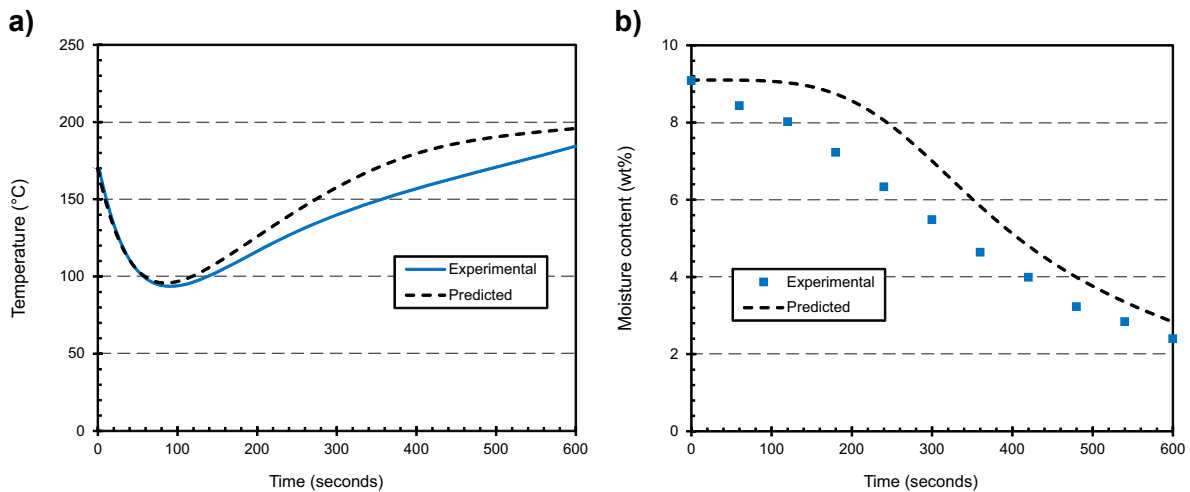


Figure 5.6: Sch_T_HDX model fit to experimentally determined a) roast profile and b) moisture content, for a 10 minute roast at a start roast temperature of 170 °C.

The best fit to experimental results for the roast profile is obtained from model Put_TX (as observed from the listed results in Table 5.4) and seen in Figure 5.7 (a) where the predicted roast profile only started to deviate from the experimental roast profile after 500 seconds, after which a slightly lower roast profile was predicted. For the higher start of roast temperatures, starting from 190 °C, the Put_TX model makes a slight underestimation at the turning point of the roast (similar to the observed underestimation by the Sch_TX and Sch_T_HDX models at the higher start of roast temperatures) and at about 200 seconds the predicted roast profile returns to the experimental results. The same lower roast profile prediction at about 500 seconds, as observed in Figure 5.7 (a), is seen however this start to happen at about 400 seconds. Indicating that for the higher roast start temperatures, the Put_TX model makes a slight underestimation of the roast profile. The moisture content prediction, as seen in Figure 5.7 (b), made the same overestimation from the start as observed by the Sch_TX and Sch_T_HDX models, however as discussed above the Put_TX model made the highest overestimation (as seen from the listed results in Table 5.5). The same was observed for all other start of roast temperatures. The predicted moisture content by this model is not as good as the Sch_T_HDX model's prediction.

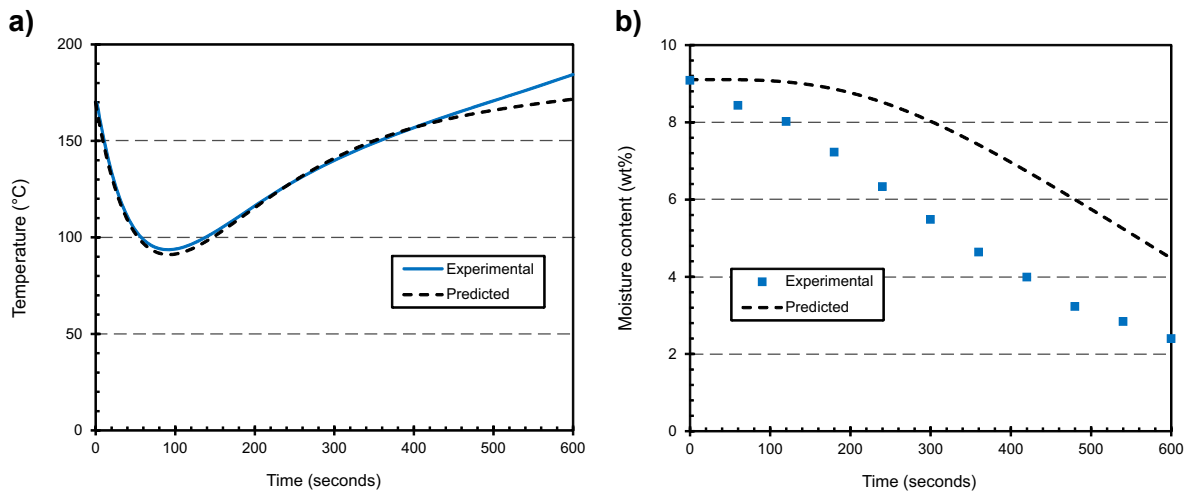


Figure 5.7: Put_TX model fit to experimentally determined a) roast profile and b) moisture content, for a 10 minute roast at a start roast temperature of 170 °C.

A further investigation of the suitability and accuracy of the three proposed models are conducted in Section 5.2, by investigation the models predictive capability in terms of roast operations lasting longer than 10 minutes.

5.2 Roasting until second crack

5.2.1 Roasting process experimental results

Batches of 4 kg of raw green coffee beans were again roasted at a start roast temperature of 170 °C to 240 °C until the second crack was reached. In Figure 5.8, the roast profiles for roasts

starting at 170 °C, 200 °C and 240 °C are presented. The roasting profiles, moisture content determination during the roasting process and the determined roasting properties for all the conducted roasts can be found in Appendix G.

From Figure 5.8, it is observed that the same roast temperatures can be reached starting from different start of roast temperatures if the roasting time is varied. From this, it can be concluded that the same degree of roast can be obtained even if a different roasting procedure (HTST or LTLT) is used.

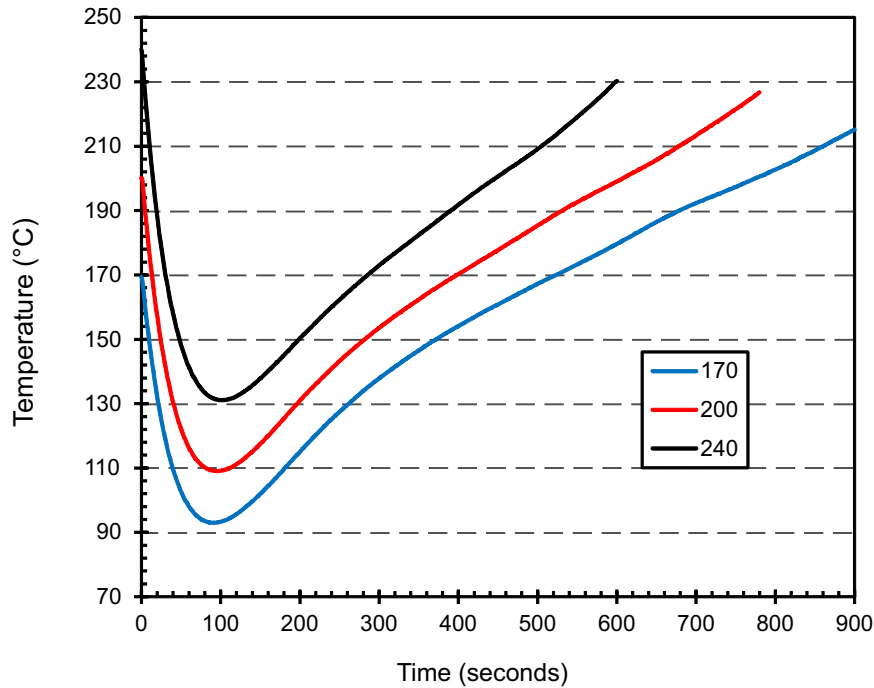


Figure 5.8: Roast profiles of coffee roasted until the second crack is reached at various temperatures.

In Figure 5.9, the moisture content determined during the roasting process, which was continued until the second crack was reached, for roasts starting 170 °C, 200 °C and 240 °C are shown. As can be seen from Figure 5.9, the moisture content of the coffee beans decreased from 9.1 to about 1.5 wt%, which is similar to results obtained by Budryn *et al.* (2012); Franca *et al.* (2005) and Schenker *et al.* (2002). As the roast start temperature is increased, the rate at which moisture is lost is also increased, resulting in a faster drying for the higher start of roast temperatures. This is also reflected in the roasting properties listed in Table 5.6, where the roasting times to reach the second crack are lower at the higher start of roast temperatures than the lower start of roast temperatures. Since all seven experimental roasts, conducted at different start of roast temperatures, were continued until the second crack was reached, all seven roasts can be classified as dark roasts. This is corroborated by the results listed in Table 5.6, where the RL for all roasts were higher than 17 % and the determined final moisture content ranged between 1 wt% and 2 wt%. All end of roast

temperatures were above 200 °C, confirming that, as stated in Section 5.1.1, the end of roast temperature can be used as another variable in qualifying the degree of roast.

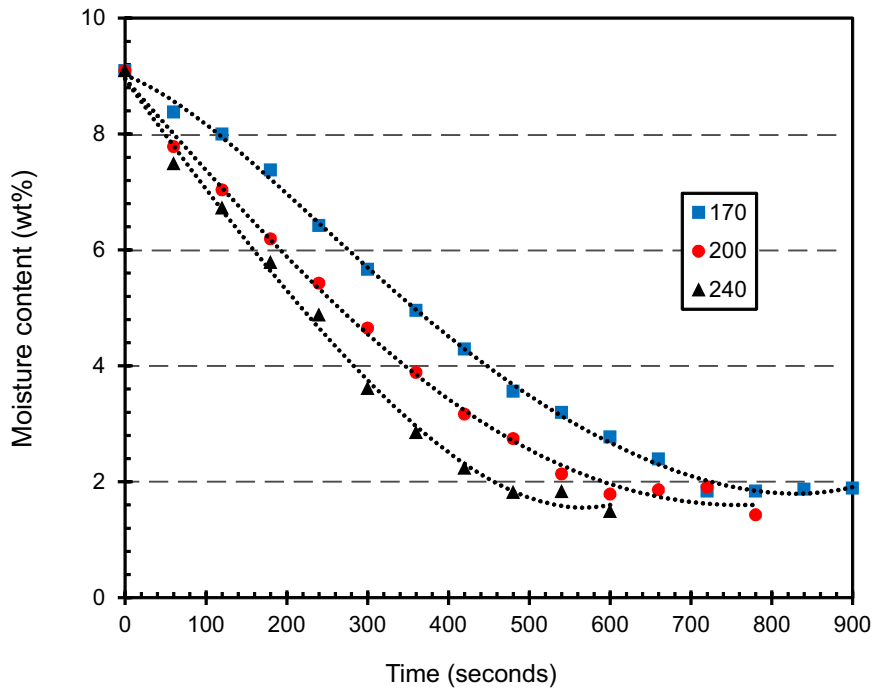


Figure 5.9: Moisture content, for roasts until the second crack is reached, of coffee for various temperatures.

From the RL reported in Table 5.6, it is observed that the higher start of roast temperature resulted in a higher RL % (the RL % at 170 °C was 17.3 %, whereas the RL % at 240 °C was 21.4 %). These results match those reported by Schenker (2000), that higher roasting temperatures at shorter roasting time (or otherwise known as the HTST roasting procedure) will result in a higher RL %.

Table 5.6: Roasting properties determined for the various roast start temperatures, for roasts continued until the second crack are reached.

Roast start temp (°C)	Roast loss (%)	Final moisture content (wt%)	Roast end temp (°C)	Roasting time (s)
170	17.3	1.89	215	900
180	17.3	1.53	208	900
190	17.9	1.13	210	900
200	21.0	1.43	227	780
210	19.2	1.37	217	780
220	19.5	1.60	225	660
230	19.0	1.76	213	660
240	21.4	1.45	230	600

Schenker (2000) concluded that the loss of dry matter was controlled more by the roasting temperature than the roasting time.

The temperatures at which the first and second crack was first observed, including when the first crack ended, as well as the time into the roasting process these occurred, are presented in Table 5.7. From Table 5.7, it can be observed that regardless of the time it took to reach it, the first crack for all roast profiles starts around 175 °C or higher, which is consistent with values reported by Gloess *et al.* (2014), and ended when the roast reached temperatures in the order of between 190 °C and 200 °C. The second crack started just as the bean batch reaches temperatures higher than 200 °C. This phenomenon was also described by Gloess *et al.* (2014). The time it takes the bean batch to go from the first crack to the second crack is seen to be decreased as a higher start of roast temperature is used. From Table 5.7, it can be seen that for the 170 °C roast it takes 50 seconds from the end of the first crack to the beginning of the second crack, whereas for the 240 °C start-off temperature, it takes 26 seconds from the end of the first crack to the beginning of the second crack. This is obviously due to the higher heating rate that takes place at the higher start of roast temperatures, as illustrated in Figure 5.8. From this it is concluded that, if the start of roast temperature is chosen high enough, the second crack will start while the first crack is still ongoing.

Table 5.7: Temperature and roasting time for when the first and second crack occurs for roasts continues until the second crack.

Roast start temp (°C)	Start first crack		End first crack		Start second crack	
	Temp (°C)	Time (s)	Temp (°C)	Time (s)	Temp (°C)	Time (s)
170	182	615	198	753	203	803
180	175	590	192	750	197	800
190	172	531	192	723	200	802
200	179	457	202	623	204	635
210	180	493	201	668	205	701
220	181	398	206	558	210	581
230	179	408	201	568	205	597
240	181	343	206	482	211	508

5.2.2 Roasting and moisture content model validation

Modelling of the roasting process was conducted with the proposed models, i.e. Sch_TX, Sch_T_HDX and Put_TX. The same roasting conditions and parameters that are listed in Table 5.3, are used during the modelling of roasts continued until the second crack, however,

the roasting temperatures are changed to those reported in Table 5.6 for every start of roast temperature.

Using the above-mentioned parameters and equations, the roast profile and moisture content are modelled for the given roasting conditions, as described in Chapter 4. In Table 5.8 and Table 5.9, the statistical performance parameters (as described in Section 4.4) that were calculated for the predicted roast profile and moisture content respectively, are listed for all start of roast temperatures and the three proposed models. The same values determined for the adjusted surface area and mass transfer coefficient, reported in Section 5.1.2, are used to ensure a better fit of the Put_TX model.

From the results presented in Table 5.8 and Table 5.9, it is observed that overall, all three models exhibit a fairly good fit to experimental results. All coefficients of determination, R^2 values are in excess of 0.7, and as discussed in Section 4.4, this indicates a good correlation between the predicted and experimental results, further implying that all three models can sufficiently predict the roast profile and moisture content for the given roasting conditions.

Table 5.8: Statistical fitting efficiency parameters determination for predicted roast profile of the three proposed models, for roasts continued until the second crack was reached.

Roast start temp (°C)	Sch_TX			Sch_T_HDX			Put_TX		
	R^2	RSME	MRE	R^2	RSME	MRE	R^2	RSME	MRE
170	0.974	12.0	7.15	0.941	15.1	8.13	0.954	12.0	4.26
180	0.960	19.0	11.3	0.916	22.2	13.2	0.941	9.53	4.72
190	0.947	15.6	8.66	0.905	18.3	9.93	0.936	10.7	4.40
200	0.951	11.7	5.88	0.913	14.7	7.27	0.935	15.1	5.24
210	0.940	13.3	6.82	0.895	16.1	8.14	0.933	12.1	4.75
220	0.921	7.09	3.44	0.927	10.5	5.02	0.930	19.1	9.02
230	0.927	13.1	6.29	0.886	15.5	7.47	0.951	11.0	4.90
240	0.957	8.5	4.04	0.920	11.1	5.27	0.932	17.3	8.12

As can be seen in Table 5.8, only for the start of roast temperature of 220, the Put_TX model had the highest obtained values for the RSME and MRE (19.1 °C and 9.02% respectively, compared to Sch_TX's 7.09 °C and 3.44 %, and Sch_T_HDX's 10.5 °C and 5.02 %) Yet for the other temperatures, the Put_TX model had the best overall fit to experimental results obtained for the roast profile, as illustrated by the results listed in Table 5.8. However, the difference in the obtained values for the RSME and MRE for all three models is not very great (as seen by the results presented in Table 5.8), implying that all three models can adequately predict the roast profile for longer roasting times.

For the shorter roasting time (as observed from results listed in Table 5.5), the Put_TX had the largest error for the predicted moisture content (highest error of 165 %) compared to Sch_TX (highest error of 113 %) and Sch_t_HDX (highest error of 73.1 %). However, the errors obtained by the Put_TX model for the predicted moisture content was fairly close to those obtained by the Sch_TX and Sch_T_HDX. From Table 5.9, it can be seen that the highest obtained values for the RSME and MRE, were 2.54 wt% and 77.6 % respectively, compared to Sch_TX's 1.88 wt% and 44.2 %, and Sch_T_HDX's 1.11 wt% and 21.4 %. From this, it is concluded that all three models make more accurate predictions at longer roasting times.

Table 5.9: Statistical fitting efficiency parameters determination for predicted moisture content of the three proposed models, for roasts continued until the second crack was reached.

Roast start temp (°C)	Sch_TX			Sch_T_HDX			Put_TX		
	R ²	RSME	MRE	R ²	RSME	MRE	R ²	RSME	MRE
170	0.910	1.58	32.8	0.972	0.79	13.6	0.889	1.66	40.6
180	0.930	1.79	43.4	0.962	1.01	18.8	0.886	1.99	55.8
190	0.815	1.81	42.0	0.919	1.03	18.4	0.843	2.00	54.1
200	0.891	1.68	32.6	0.952	1.04	17.9	0.822	2.07	52.6
210	0.885	1.79	41.9	0.956	1.04	19.9	0.811	2.19	60.3
220	0.752	1.88	44.2	0.951	1.11	21.4	0.819	2.54	77.6
230	0.909	1.46	27.0	0.963	0.890	15.5	0.840	2.15	56.1
240	0.881	1.76	33.7	0.945	1.14	19.1	0.812	2.53	74.5

The results obtained from modelling the roasting process that was continued until the second crack, for a roast start temperature of 170 °C, are shown in Figure 5.10 to Figure 5.12, where the predicted roast profile and moisture content are compared to experimental results. The results obtained for the other start of roast temperatures can be seen in Appendix H.

From Figure 5.10 (a), it can be seen that the Sch_TX model's prediction for longer roasts showed the same behaviour as the predicted results for shorter roast (shown in Figure 5.5 (a)), where a slight overestimation of the roast profile can be observed from around 100 seconds into the roasting process. At the higher start of roast temperatures (210 to 240 °C), the same deviation from the start of the roast where the Sch_TX model underestimated the roast profile at the turning point of the roast profile for the 10 minute roasts, were observed for the longer roasts. After about 160 seconds the predicted model showed the same overestimation as observed for the 10 minute roasts. The moisture content prediction, as seen in Figure 5.10 (b), made a better overall estimation than the one predicted for the shorter

roasting time (as can be seen in Figure 5.5 (b)). However, the overestimation at the start of the roasting process is still present, indicating that the Sch_TX model assumes a slower drying rate than the drying rate experimentally observed. The same was observed for all other start of roast temperatures.

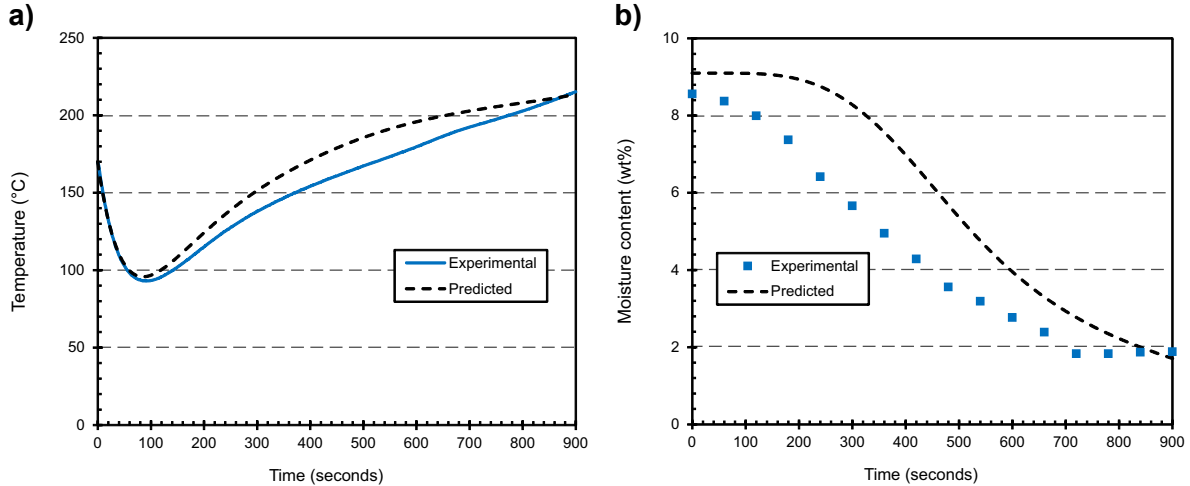


Figure 5.10: Sch_TX model fit to experimentally determined a) roast profile and b) moisture content, for a 15 minute roast at a start roast temperature of 170 °C.

The same is found for the Sch_T_HDX model predicted roast profile, as seen in Figure 5.11 (a), however a slightly higher overestimation of the roast profile can be observed from around 100 seconds into the roasting process. At the higher start of roast temperatures, the same deviation from the start of the roast where the Sch_T_HDX model underestimated the roast profile at the turning point of the roast profile for the 10 minute roasts, were observed for the longer roasts. After which the predicted model showed the same overestimation as observed for the 10 minute roasts.

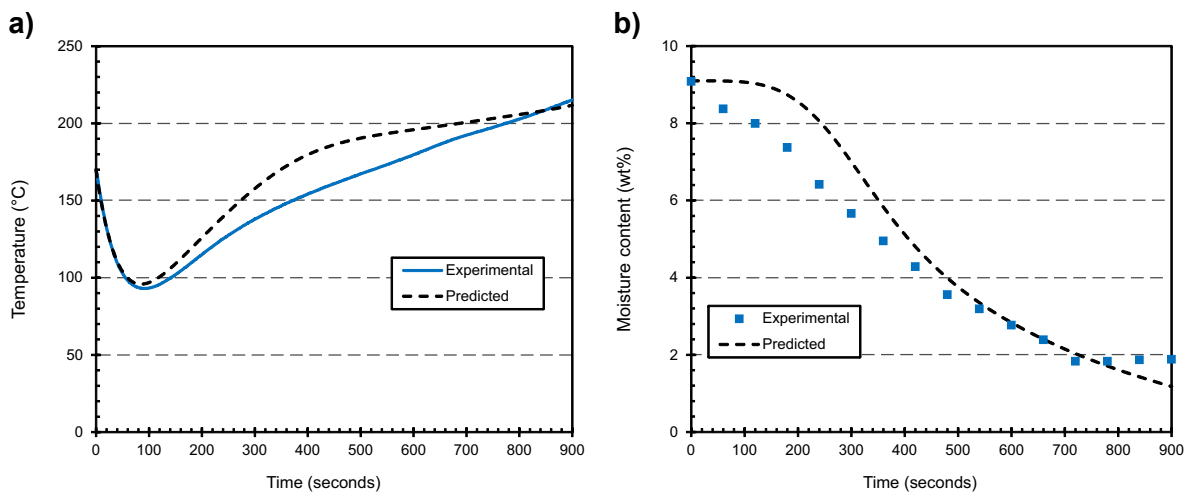


Figure 5.11: Sch_T_HDX model fit to experimentally determined a) roast profile and b) moisture content, for a 15 minute roast at a start roast temperature of 170 °C.

The moisture content prediction, as seen in Figure 5.11 (b), made a better overall estimation than the one predicted for the shorter roasting time (as can be seen in Figure 5.6 (b)). Where, after 600 seconds, the moisture content prediction came fairly close to the experimental results, which is reflected in the results obtained from Table 5.9 for the longer roasts compared to the results obtained from Table 5.5 for the 10 minute roasts. Compared to the Sch_TX model, the predicted drying rate is a bit faster resulting in a more accurately predicted moisture content (which is also visible in the results listed in Table 5.9). The same behaviour was observed for all other start of roast temperatures.

The roast profile prediction of the Put_TX model for the roast start temperature of 170 °C is shown in Figure 5.12 (a). Here, the same behaviour as seen with the 10 minute roast are observed where the predicted roast profile only started to deviate from the experimental roast profile after 500 seconds, after which an underestimation of the roast profile is predicted. The same underestimation at the turning point of the roast that was observed for the 10 minute roast at higher temperatures are observed for the longer roasting times as well. However, at the higher roasting temperatures, the predicted model does not converge with the experimental results as seen for the 10 minute roast at about 200 seconds but keeps on underestimation the roast profile. The moisture content prediction, as seen in Figure 5.12 (b), had a better overall prediction for the longer roasting times compared to the 10 minute roasts. There still exist an overestimation from the start, however to the end of the roast the predicted values are closer to the experimental ones and at about 800 seconds the predictive values start to underestimate the moisture content. The same was observed for the other start of roast temperatures, except at the higher temperatures (starting from 220 °C) where the underestimation at the end of the roast does not occur.

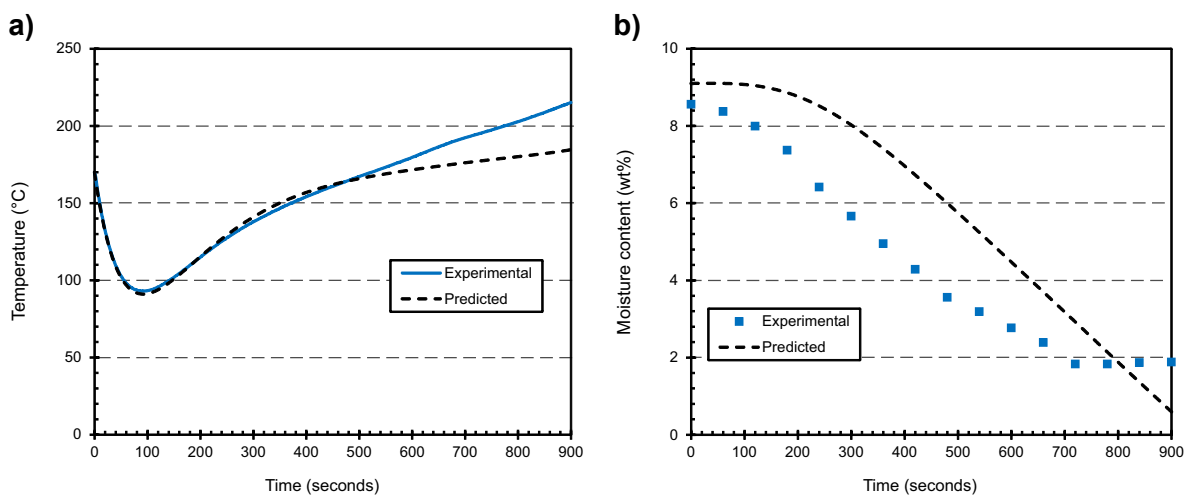


Figure 5.12: Put_TX model fit to experimentally determined a) roast profile and b) moisture content, for a 15 minute roast at a start roast temperature of 170 °C.

A further investigation of the suitability and accuracy of the three proposed model are conducted in Section 5.3 by investigation the models' predictive capability in terms of roasts conducted with moisture increased coffee beans.

5.3 Roasting with moisture increased green beans

5.3.1 Roasting process experimental results

Batches of 4 kg moisture increased raw green coffee beans were roasted, at a start-off roast temperature of 170 to 230 °C until the second crack was reached. The increased moisture content resulted in coffee beans with initial moistures contents of 12.7 wt%, 13.3 wt% and 14.5 wt% moisture. The roast profiles of coffee roasted at 170 °C, determined for different initial moisture contents are shown in Figure 5.13. From Figure 5.13, it can be observed that at higher initial moisture contents, a lower heating rate is achieved compared to lower initial moisture contents at the same start roast temperature. This is due to the fact that more heat is needed to evaporate the extra moisture inside the beans. Therefore, at the higher initial moisture content, most of the heat transferred is first used for evaporation until enough moisture have been released from the bean. The roasting profiles, moisture content determination during the roasting process and the determined roasting properties for all the conducted roasts can be found in Appendix G.

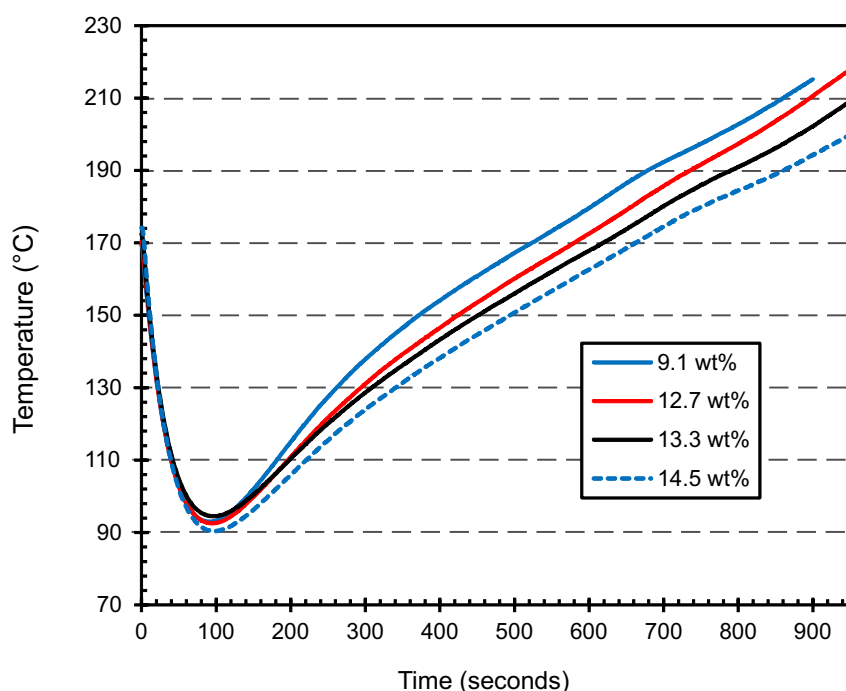


Figure 5.13: Roast profiles of coffee roasted at 170 °C until the second crack is reached, at various initial moisture content.

In Figure 5.14, the different moisture contents determined during the roasting process for the various moisture increased coffee beans, which was continued until the second crack was reached, for a roast starting temperature of 170 °C are shown. These findings shown in Figure

5.14 agrees with those reported by Schenker (2000) (as seen in Figure 4.7), where the higher initial moisture content shows a faster drying rate than the lower initial moisture content beans.

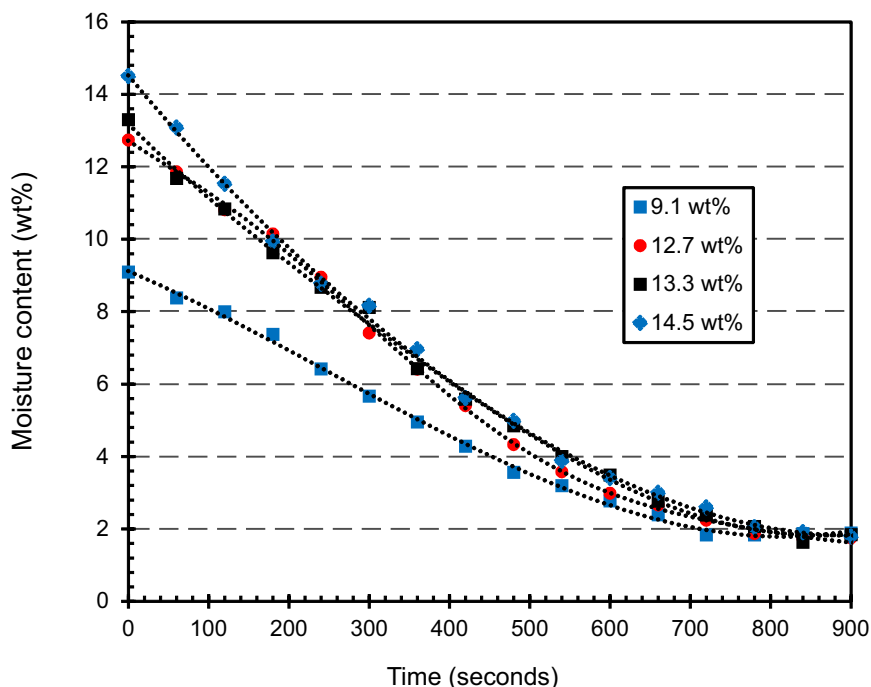


Figure 5.14: Moisture content, for roasts until the second crack is reached, of coffee for various temperatures.

The results listed in Table 5.10, represents the roasting properties determined for the 12.7 wt% initial moisture content coffee beans, at the four roast start temperatures. As the roast start-off temperatures are increased, the rate at which moisture is lost is also increased, resulting in a faster drying for the higher start of roast temperatures. This is observed in the roasting properties listed in Table 5.10, where the roasting times to reach the second crack are lower at the higher start of roast temperatures than the lower start of roast temperatures. Since all four experimental roasts, conducted at different start of roast temperatures, were continued until the second crack was reached, all four roast can be classified as dark roasts.

Table 5.10: Roasting properties determined for the various roast start temperatures, for roasts conducted with 12.7 wt% moisture content coffee beans.

Roast start temp (°C)	Roast loss (%)	Final moisture content (wt%)	Roast end temp (°C)	Roasting time (s)
170	22.4	1.56	219	960
190	19.9	1.85	213	900
210	22.7	1.67	221	720
230	21.5	1.93	219	660

This is corroborated by the results listed in Table 5.6, where the RL for all roasts were higher than 17 % and the determined final moisture content ranged between 1 wt% and 2 wt%. All end of roast temperatures were above 200 °C, indicating that, as stated in Section 5.1.1, the end of roast temperature can be used as another variable in identifying the degree of roast.

The temperatures at which first and second crack were first observed, including when the first crack ended, as well as the time into the roasting process these occurred, are presented in Table 5.11. From Table 5.11, it can be observed that regardless of the change in initial moisture content, the first crack for all roast profiles started at about 175 °C or higher, which is consistent with the values found for the previous roasts at various roasting times and start roast temperatures. The first crack ended when the roasts reached between 190 °C and 200 °C, while the second crack started just as the bean batch reached temperatures higher than 200 °C. From these results, and the results found for the previous roasts, it can be concluded that using these temperature ranges found for the first and second crack, the degree of roast can be predicted from the temperature progression of the roast profile and end of roast temperatures.

Table 5.11: Temperature and roasting time for when the first and second crack occurs, for roast conducted with 12.7 wt% moisture content coffee beans.

Roast start temp (°C)	Start first crack		End first crack		Start second crack	
	Temp (°C)	Time (s)	Temp (°C)	Time (s)	Temp (°C)	Time (s)
170	179	648	196	789	203	847
190	177	604	195	754	203	825
210	176	459	203	628	204	637
230	176	413	203	580	206	597

5.3.2 Roasting and moisture content model validation

Modelling of the roasting process was conducted with the proposed models, i.e. Sch_TX, Sch_T_HDX and Put_TX.

When the moisture content of the beans was increased, the beans absorbed an amount of water which resulted in the bean's weight to increase. Along with the increased weight, the beans also had an expansion in size to accommodate the absorbed water. This resulted in an increased bean diameter and consequently an increased bean surface area. Therefore, in order to accurately model the experimental roast conducted, the roasting conditions and parameters for the increased moisture content beans needs to be determined. In Table 5.12, the roasting conditions and parameters for the various experimental roasts, determined as described in Chapter 3, are listed.

Table 5.12: Roasting conditions and parameters determined for the moisture increased coffee beans.

Parameter	Value
A_b	4.02, 4.19, 4.28 m ² *
d_b	7.27×10^{-3} , 7.52×10^{-3} , 7.87×10^{-3} m
G_g	0.047 kg/s
$m_{b(d.b)}$	3.49, 3.47, 3.42 kg _{d.b.}
$RH_{g,i}$	0.1 %
$T_{b,i}$	20 °C
$T_{g,i}$	See Appendix G
$T_{rp,i}$	170 - 230 °C (at 20 °C intervals)
t	See Table 5.10, Appendix G
v_g	0.6 m/s
$X_{b,i}$	0.127, 0.133, 0.145 kg/kg _{d.b.}

Using the above-mentioned parameters and equations, the roast profile and moisture content are modelled for the given roasting conditions, as described in Chapter 4. In Table 5.4 and Table 5.5, the goodness of fit values (as described in Section 4.4) that were calculated for the predicted roast profile and moisture content respectively, are listed for all start of roast temperatures and the three proposed models. The values determined for the adjusted surface area and mass transfer coefficient, reported in Section 5.1.2, are used to ensure a better fit of the Put_TX model.

Table 5.13: Statistical fitting efficiency parameters determination for predicted roast profile of the three proposed models, for roasts conducted with 12.7 wt% moisture content coffee beans.

Roast start temp (°C)	Sch_TX			Sch_T_HDX			Put_TX		
	R ²	RSME	MRE	R ²	RSME	MRE	R ²	RSME	MRE
170	0.893	23.2	13.6	0.911	22.1	13.4	0.934	14.8	4.09
190	0.879	24.2	12.4	0.901	22.9	12.3	0.933	13.2	5.00
210	0.867	25.3	12.1	0.898	23.2	11.7	0.931	14.4	5.22
230	0.861	25.1	11.4	0.898	22.6	10.9	0.962	14.5	7.65

From the results presented in Table 5.13 and Table 5.14, it is observed that overall, all three models had a fairly good fit to experimental results. All coefficient of determination, R²-values were larger than 0.7, and as discussed in Section 4.4, this indicates a good correlation

between the predicted and experimental results, further implying that all three models can sufficiently predict the roast profile and moisture content for the given roasting conditions.

The same behaviour as observed in Section 5.1.2 and 5.2.2, is observed in Table 5.13 and Table 5.14, where the Put_TX model, had the best fit to experimental results obtained for the roast profile. The moisture content prediction, however, had higher errors (127 %) than those compared to Sch_TX (highest error of 31.7 %) and Sch_t_HDX (highest error of 30.7 %). From Figure 5.15 and Figure 5.17, it can be seen that these high errors are due to an overestimation of the predicted moisture content, where the Put_TX model exhibited the highest degree of overestimation of the predicted moisture content.

Table 5.14: Statistical fitting efficiency parameters determination for predicted moisture content of the three proposed models, for roasts conducted with 12.7 wt% moisture content coffee beans.

Roast start temp (°C)	Sch_TX			Sch_T_HDX			Put_TX		
	R ²	RSME	MRE	R ²	RSME	MRE	R ²	RSME	MRE
170	0.931	1.80	18.6	0.954	1.58	24.0	0.834	3.46	89.0
190	0.847	2.02	21.3	0.904	1.80	25.7	0.873	3.71	96.8
210	0.885	2.33	26.9	0.911	2.16	30.7	0.796	4.44	127
230	0.908	2.02	31.7	0.933	1.76	21.6	0.819	4.16	106

The results obtained from modelling the roasting process for a 12.7 wt% moisture content coffee bean batch, continued until the second crack, for a roast start temperature of 170 °C, are shown in Figure 5.15 and Figure 5.17. Here, the predicted roast profile and moisture content are compared to experimental results. The results obtained for the other start of roast temperatures and initial moisture content coffee beans can be seen in Appendix H.

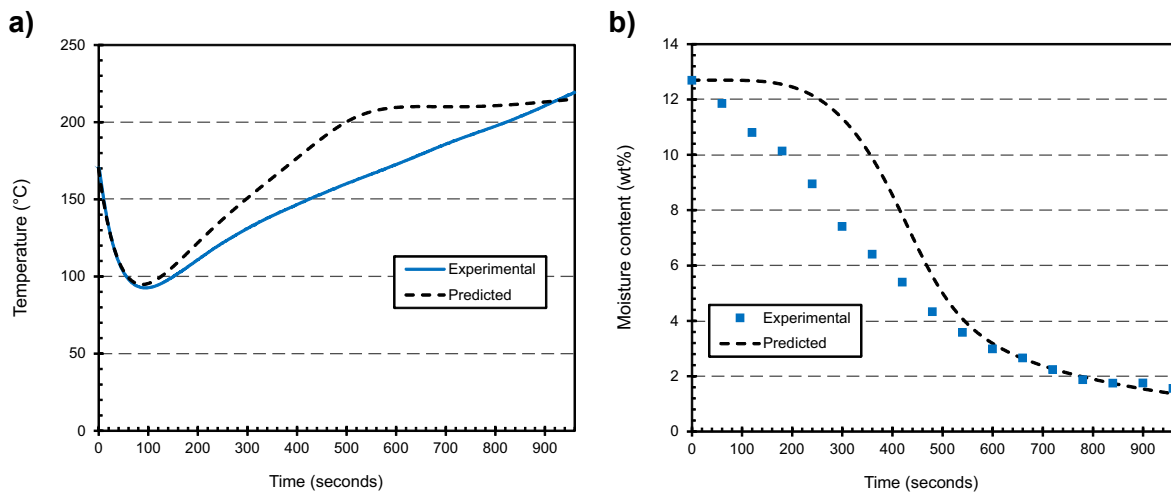


Figure 5.15: Sch_TX model fit to experimentally determined a) roast profile and b) moisture content, for 12.7 wt% moisture content coffee beans roasted at a start roast temperature of 170 °C.

The peaks that can be seen in Figure 5.15 (a) and Figure 5.16 (a) at about 500 seconds, is the direct result of the moisture loss model behaviour to higher moisture contents. In Section 4.6.1, it was concluded that, due to the empirical nature of the two proposed moisture loss models, the models are sensitive to higher moisture contents. At higher moisture contents, the predicted moisture content will show a steeper drying rate slope than observed in experimental results which directly influence the bean temperature. The influence on the bean temperature can be ascribed to the moisture loss occurring at a faster rate, according to the model, which allows for the beans to have a faster heat transfer rate, resulting in a faster rise in bean temperature. This faster rise in bean temperature is then transferred to the predicted roast profile, resulting in predicted roast profiles as observed in Figure 5.15 (a) and Figure 5.16 (a). The same behaviour is seen for the other start of roast temperatures. The same underestimation at the start of the roast, which was observed for the higher temperatures at both roasting times for the Sch_TX and Sch_T_HDX models, is seen for the 230 °C roast profile. However, here the underestimation was only with about 2 °C, compared to the higher difference found for the other roasting times (about 10 °C).

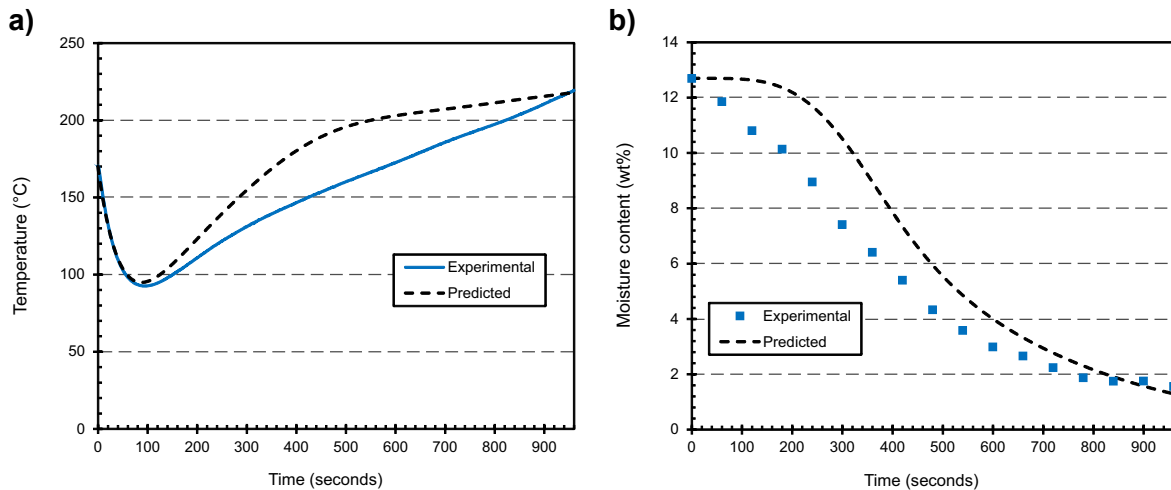


Figure 5.16: Sch_T_HDX model fit to experimentally determined a) roast profile and b) moisture content, for 12.7 wt% moisture content coffee beans roasted at a start roast temperature of 170 °C.

For the increased moisture content, the roast profile predicted by the Put_TX (as seen in Figure 5.17 (a)) model started to deviate from the experimental roast profile much quicker than those obtained previously (400 seconds compared to 500). The same behaviour observed for the long roasting times, where at the higher temperatures the roast profile was entirely underestimated, is observed here for the higher roasting temperatures. Indicating that the Put_TX model roast profile predictions handled the increase in initial moisture content better than those predicted by Sch_TX and Sch_T_HDX, and showed the same behaviour for the same roasting conditions, regardless of the initial moisture content. The moisture content prediction, as seen in Figure 5.17 (b), showed the same overestimation at the start of the roast

than the other roasting times, however the underestimation at the end of the roasting process is not observed for the lower roasting temperatures. At the higher roasting temperatures, the moisture content model, ended with an overestimated value of about 2 wt%, indicating that the Put_TX model assumes a slower drying rate for the higher roasting temperatures. This indicates that, although the Put_TX model can adequately account for the increased in initial moisture content, it does not account for an increase in roasting temperature when predicting the moisture content (the same behaviour was observed for the other roasting times, however there the final predicted moisture content was fairly close to the experimental values). For the higher the inlet air temperature, the faster the moisture will evaporate from the beans (Burmester & Eggers, 2010).

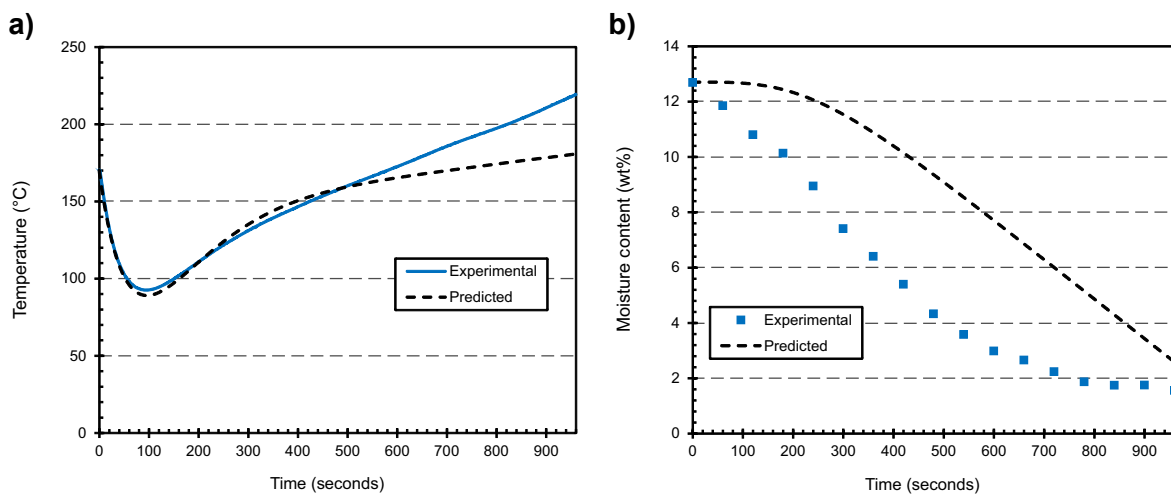


Figure 5.17: Put_TX model fit to experimentally determined a) roast profile and b) moisture content, for 12.7 wt% moisture content coffee beans roasted at a start roast temperature of 170 °C.

The results listed in Table 5.15 and Table 5.16, are the statistical performance parameters determined for the predicted roast profile and moisture content, at roasting with coffee beans consisting of a 13.3 wt% initial moisture content.

Table 5.15 Statistical fitting efficiency parameters determination for predicted roast profile of the three proposed models, for roasts conducted with 13.3 wt% moisture content coffee beans.

Roast start temp (°C)	Sch_TX			Sch_T_HDX			Put_TX		
	R ²	RSME	MRE	R ²	RSME	MRE	R ²	RSME	MRE
170	0.892	25.6	14.8	0.915	23.9	14.3	0.936	15.5	5.13
190	0.815	33.2	18.0	0.861	30.8	17.5	0.930	14.2	5.58
210	0.813	28.1	14.9	0.866	26.0	14.4	0.917	15.6	5.73
230	0.757	32.5	15.4	0.815	29.6	14.7	0.902	16.8	7.11

The same behaviour as shown for the 12.7 wt% moisture content predictions (discussed in Table 5.13 and Table 5.14) can be observed here. The Put_TX model had a better overall fit

to experimental roast profiles, but the worst fit to experimental moisture content. This is observed for all roasting temperatures.

Table 5.16: Statistical fitting efficiency parameters determination for predicted moisture content of the three proposed models, for roasts conducted with 13.3 wt% moisture content coffee beans.

Roast start temp (°C)	Sch_TX			Sch_T_HDX			Put_TX		
	R ²	RSME	MRE	R ²	RSME	MRE	R ²	RSME	MRE
170	0.910	2.25	23.6	0.932	2.11	32.4	0.846	3.09	64.6
190	0.880	1.95	26.9	0.917	1.78	22.2	0.875	3.36	74.3
210	0.901	2.21	22.9	0.924	2.11	32.1	0.817	3.42	79.9
230	0.896	2.03	33.0	0.919	1.91	23.4	0.803	3.73	102

The results listed in Table 5.15 and Table 5.16, the statistical performance parameters determined for the predicted roast profile and moisture content, at roasting with coffee beans consisting of a 14.5 wt% initial moisture content.

Table 5.17: Statistical fitting efficiency parameters determination for predicted roast profile of the three proposed models, for roasts conducted with 14.5 wt% moisture content coffee beans.

Roast start temp (°C)	Sch_TX			Sch_T_HDX			Put_TX		
	R ²	RSME	MRE	R ²	RSME	MRE	R ²	RSME	MRE
170	0.831	35.0	22.3	0.890	32.1	21.0	0.933	12.8	4.43
190	0.830	31.4	18.2	0.890	28.4	17.1	0.923	13.6	5.06
210	0.767	37.6	19.1	0.862	33.8	18.0	0.921	14.4	5.68
230	0.671	34.7	16.4	0.792	31.0	15.6	0.888	19.3	8.47

The same behaviour as shown for the 12.7 wt% moisture content predictions (as summarised in Table 5.13 and Table 5.14) can be observed here. The Put_TX model again showed a better overall fit to experimental roast profiles but was the worst performer in fitting its predicted moisture content to experimentally obtained moisture content. This is observed for all roasting temperatures.

Table 5.18: Statistical fitting efficiency parameters determination for predicted moisture content of the three proposed models, for roasts conducted with 14.5 wt% moisture content coffee beans.

Roast start temp (°C)	Sch_TX			Sch_T_HDX			Put_TX		
	R ²	RSME	MRE	R ²	RSME	MRE	R ²	RSME	MRE
170	0.904	2.39	22.1	0.920	2.45	35.1	0.836	3.73	76.3
190	0.821	2.37	20.8	0.877	2.43	35.8	0.886	3.65	73.7
210	0.894	2.46	35.0	0.920	2.31	25.3	0.833	4.15	94.5
230	0.882	2.37	38.3	0.912	2.13	24.5	0.841	3.87	80.2

5.4 Summary of modelling validation

The results obtained from the three proposed models were validated against experimental results. When modelling the roasting process conducted for 10 minutes, the Put_TX model had the best overall fit to experimental results for the roast profile. However, the moisture content prediction showed the highest degree of overestimation compared to experimental results for all three models. The Sch_TX and Sch_T_HDX models resulted in a slight overestimation of the roast profile, and of the two, the Sch_T_HDX had the best moisture content prediction.

The same results were found for the longer roasting times, where the best overall fit to experimental results was the Put_TX model. At the end of the roasting process, however, this model began to underestimate the roasting profile. The moisture content prediction had a better fit to the experimental results for the longer roasting times than those found for the 10 minute roasts, however it still resulted in the highest overestimation of the moisture content. Again, a slight overestimation of the roast profile was observed for the Sch_TX and Sch_T_HDX models, and of the two, the Sch_T_HDX had the best moisture content prediction.

For the increased initial moisture content modelling, the Put_TX model still exhibits the best overall fit to the experimental results. At the end of the roasting process, the same underestimation of the roast profile is present than for the longer roasting times. The moisture content prediction still results in an overestimated prediction. The increased initial moisture content results in a higher degree of overestimation of the roast profile, compared to the other roasts, for both the Sch_TX and Sch_T_HDX models. These higher levels of overestimation were attributed to the empirical nature of the moisture loss models, which are sensitive to variation in moisture contents. Of the two models, the Sch_T_HDX model proved to have the best moisture content prediction.

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CHAPTER 6 – Conclusion and recommendations

Overview

In this final chapter, the conclusions drawn from the results that were obtained throughout this investigation are summarised. From this, recommendations and suggestions will originate to support future work.

"I believe humans get a lot done, not because we're smart, but because we have thumbs so we can make coffee." – F. Rosenberg

6.1 Conclusion

The main objective of this study was to investigate the heat and mass transfer models proposed by various authors in literature and to determine if these models can be implemented to model the roasting process. The modelled roasting process is represented by the predicted roast profile, which is validated using experimental results.

In Chapter 4, three models were identified that could adequately model the temperature and moisture content of the beans during roasting. From Chapter 5, it was found that all three models could sufficiently predict the roast profile from the modelled bean temperature and moisture content. However, all three consistently overestimated the moisture content during roasting. For longer roasting times, the final moisture content prediction was closer to the experimental value. With the increased initial moisture content, the Sch_TX and Sch_T_HDX models resulted in higher degrees of overestimation of the roast profile. It is therefore concluded that the Sch_TX and Sch_T_HDX models are more accurate in predicting the roast profile for roasting with lower moisture content beans and further investigation into their applicability to high moisture content should be conducted. Although the roast profile modelled by Put_TX had the best overall fit to experimental results, it consistently deviated from the roast profile after 500 seconds from where it greatly underestimated the roast profile. The Sch_TX and Sch_T_HDX models continually showed a slight overestimation of the roast. However, along with the moisture loss model, the Put_TX model is concluded to be less applicable for modelling the roasting process than the Sch_TX and Sch_T_HDX models due to the fact that, once the deviation occurs, it kept moving farther away from experimental results, where the other two models seem to correct themselves once a deviation occurs.

The second objective of this study was to classify the roast degree of the beans and to investigate the possibility of predicting the roast degree from the roast profile. It was found that the occurrence of the first and second crack consistently transpired at the same temperatures. From this, it is concluded that a rudimentary roast degree prediction can be made based on the end temperatures of the roast. This is based on the temperature where the first and second crack is expected to occur.

It can be concluded that all three models can be used in the optimisation and control of the coffee roasting process due to the good correlation between the experimental and predicted results, despite some deviations, although further investigation is needed into the optimisation of the moisture loss models. This may result in a more accurate estimation of the moisture loss during roasting since there are two adjustable (or manipulated) parameters in the Put_TX model, while the Sch_TX and Sch_T_HDX models are better suited for optimisation and control.

For the purpose of predicting the roast degree from the roast profile, the Sch_TX and Sch_T_HDX models are better suited. This is due to the significantly lower difference between the experimental and predicted end temperatures. Since the Put_TX model results in a lower predicted end temperature, the estimated degree of roast could be lighter than expected. Therefore, it is recommended to further investigate the Put_TX model. From Section 4.1.2, it can be seen that the Put_TX model does not account for exothermic heat generation. This may be the cause of the lower estimated temperature, and the effect of exothermic heat generation on the bean temperature and roast profile should be further investigated.

6.2 Recommendations

The following recommendations are made for further study of the coffee roasting process and the modelling thereof:

- A more concise method needs to be investigated to determine the degree of roast online for most roast degree determination methods are conducted in hindsight, and will therefore not be of great assistance for optimisation and control of the roasting process.
- A more accurate mass transfer model should be investigated, for during roasting volatiles and dry matter are also released with the moisture of the beans. A more accurate mass loss model (instead of just moisture loss) could increase the accuracy of the bean temperature model.
- From literature, it was seen that the proposed moisture loss models could accurately predict the moisture content of small samples (and sometimes individual beans) during the roasting process. However, from the modelling conducted in Chapter 5, a consistent overestimation of the moisture content was found to exist. Further research into moisture loss that occurs during large batch roasting should be investigated, to see the impact the size of the batch has on the moisture loss that occurs.
- Optimise the available moisture loss models so that a more accurate prediction of the moisture loss during roasting can be obtained, as well as the models' sensitivity to higher moisture content.
- Further investigate the effect that exothermic roasting reactions can have on the bean temperature and whether or not it is critical in the modelling of the bean temperature and consequently the roast profile.
- Roasting experiments conducted with different green coffee beans (difference in origin, processing methods, etc.), to quantify the influence these factors will have on the roasting process and whether the models can be applied to roasting with different beans.

"I'd like to THANK whoever saw a bunch of cherries and thought...HEY!! If I dry out a bunch of those berry seeds, call them BEANS, smash them and add hot water, it will be AWESOME!" – J. Masse

Appendix A – Measured properties of green beans

A.1 Green beans

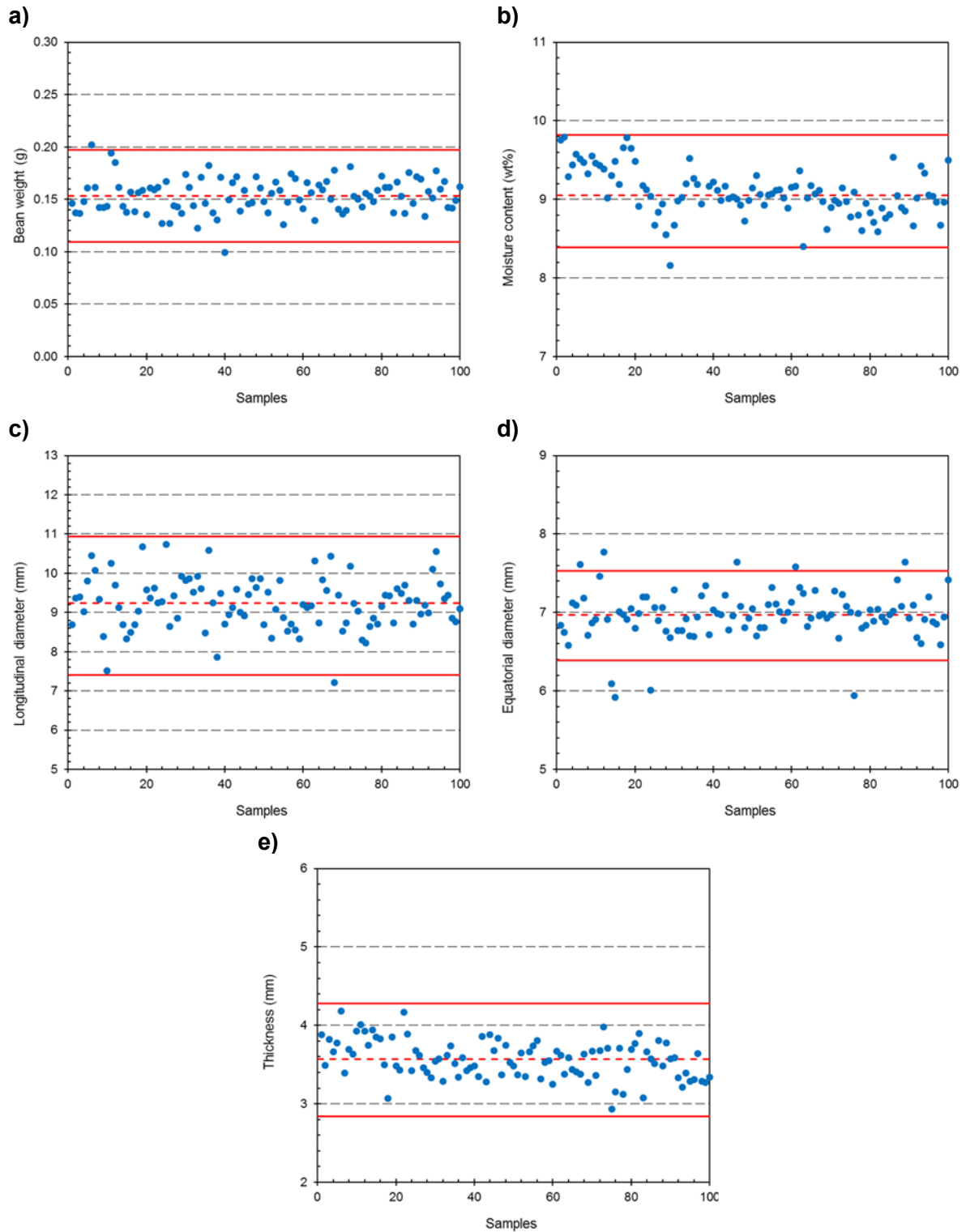


Figure A.1: Measured properties of green beans showing median, upper and lower limits of a) bean weight, b) initial moisture content, c) longitudinal diameter, d) equatorial diameter and e) thickness.

A.2 Green beans with 12.7 wt% initial moisture content

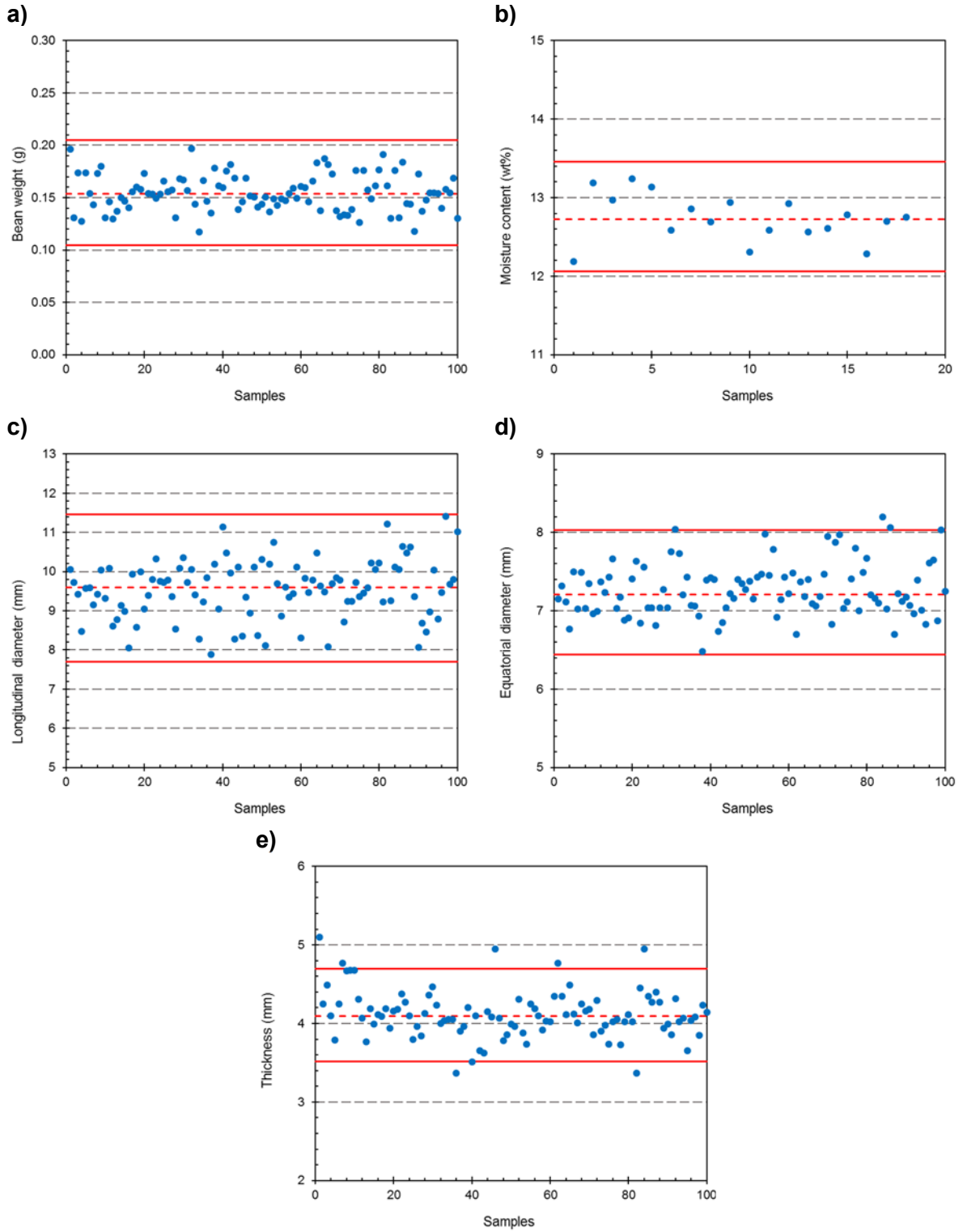


Figure A.2: Measured properties of 12.7 wt% initial moisture content green beans showing median, upper and lower limits of a) bean weight, b) initial moisture content, c) longitudinal diameter, d) equatorial diameter and e) thickness.

A.3 Green beans with 13.3 wt% initial moisture content

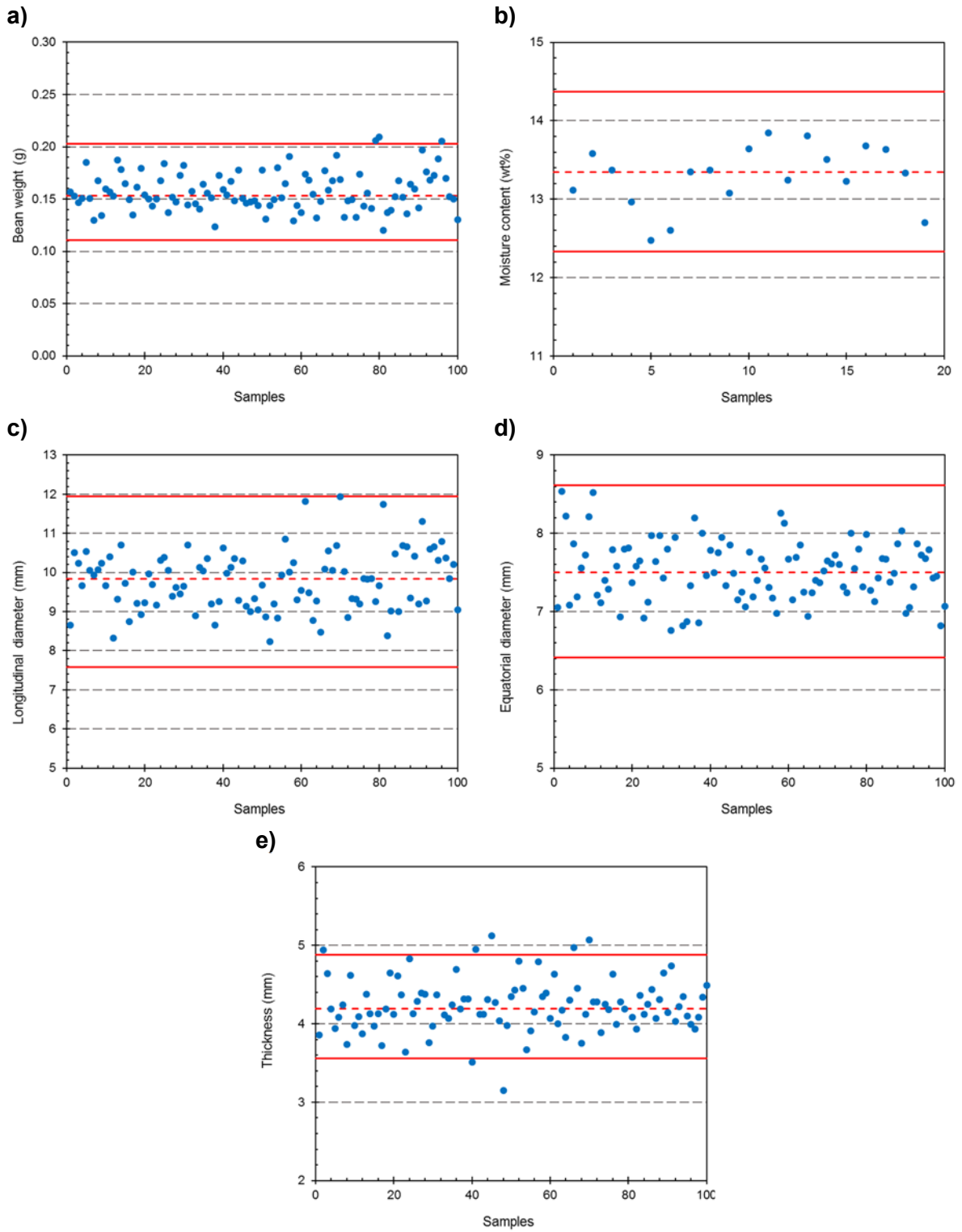


Figure A.3: Measured properties of 13.3 wt% initial moisture content green beans showing median, upper and lower limits of a) bean weight, b) initial moisture content, c) longitudinal diameter, d) equatorial diameter and e) thickness.

A.4 Green beans with 14.5 wt% initial moisture content

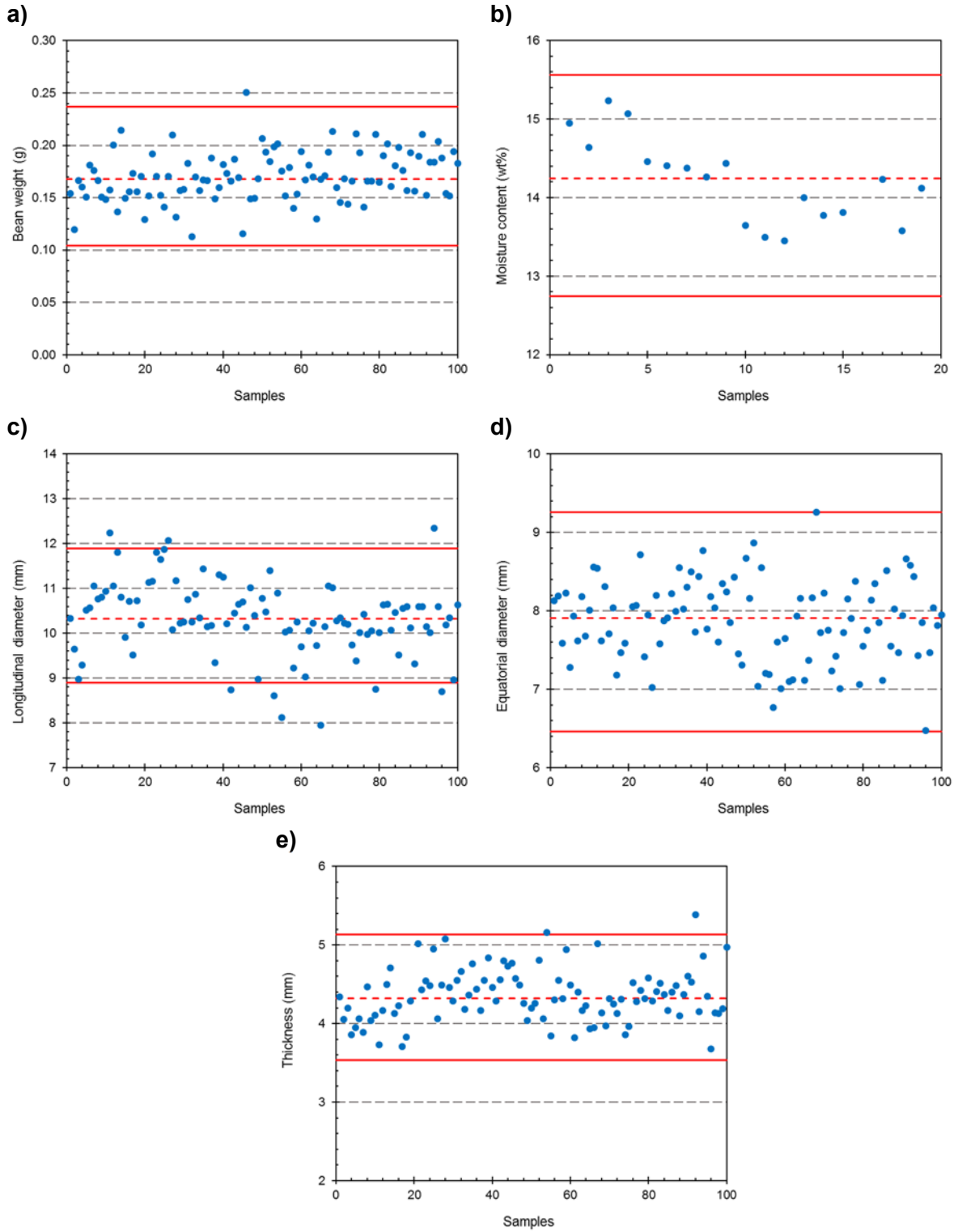


Figure A.4: Measured properties of 14.5 wt% initial moisture content green beans showing median, upper and lower limits of a) bean weight, b) initial moisture content, c) longitudinal diameter, d) equatorial diameter and e) thickness.

Appendix B – Measured roasting conditions

Table B.1: Measured roasting conditions.

Initial bean temperature	Air velocity	Air mass flow
°C	m/s	kg/s
17.4	0.6	0.0433
17.9	0.5	0.0474
20.6	0.6	0.0489
18.9	0.6	0.0484
21.8	0.7	0.0464
19.9	0.8	0.0463
21.3	0.6	0.0484
21.0	0.6	0.0469
20.1	0.6	0.0460
17.6	0.8	0.0449
16.8	0.5	0.0473
18.5	0.6	0.0472
18.2	0.4	0.0460
21	0.6	0.0449
20.7	0.6	0.0464

Appendix C – Thermophysical properties of drying air

Table C.1: Thermophysical properties of drying air (obtained from Incropera *et al.*, 2013).

Temperature	Density	Heat capacity	Viscosity	Thermal conductivity
K	kg/m ³	J/kg·K × 10 ⁻³	kg/m·s × 10 ⁷	W/m·K × 10 ³
100	3.5562	1.032	71.1	9.34
150	2.3364	1.012	103.4	13.8
200	1.7458	1.007	132.5	18.1
250	1.3947	1.006	159.6	22.3
300	1.1614	1.007	184.6	26.3
350	0.995	1.009	208.2	30
400	0.8711	1.014	230.1	33.8
450	0.774	1.021	250.7	37.3
500	0.6964	1.03	270.1	40.7
550	0.6329	1.04	288.4	43.9
600	0.5804	1.051	305.8	46.9
650	0.5356	1.063	322.5	49.7
700	0.4975	1.075	338.8	52.4
750	0.4643	1.087	354.6	54.9
800	0.4354	1.099	369.8	57.3
850	0.4097	1.11	384.3	59.6
900	0.3868	1.121	398.1	62
950	0.3666	1.131	411.3	64.3
1000	0.3482	1.141	424.4	66.7
1100	0.3166	1.159	449	71.5
1200	0.2902	1.175	473	76.3
1300	0.2679	1.189	496	82
1400	0.2488	1.207	530	91
1500	0.2322	1.23	557	100
1600	0.2177	1.248	584	106
1700	0.2049	1.267	611	113
1800	0.1935	1.286	637	120
1900	0.1883	1.307	663	128
2000	0.1741	1.337	689	137
2100	0.1658	1.372	715	147

2200	0.1582	1.417	740	160
2300	0.1513	1.478	766	175
2400	0.1448	1.558	792	196
2500	0.1389	1.665	818	222

C.1 Density of drying air

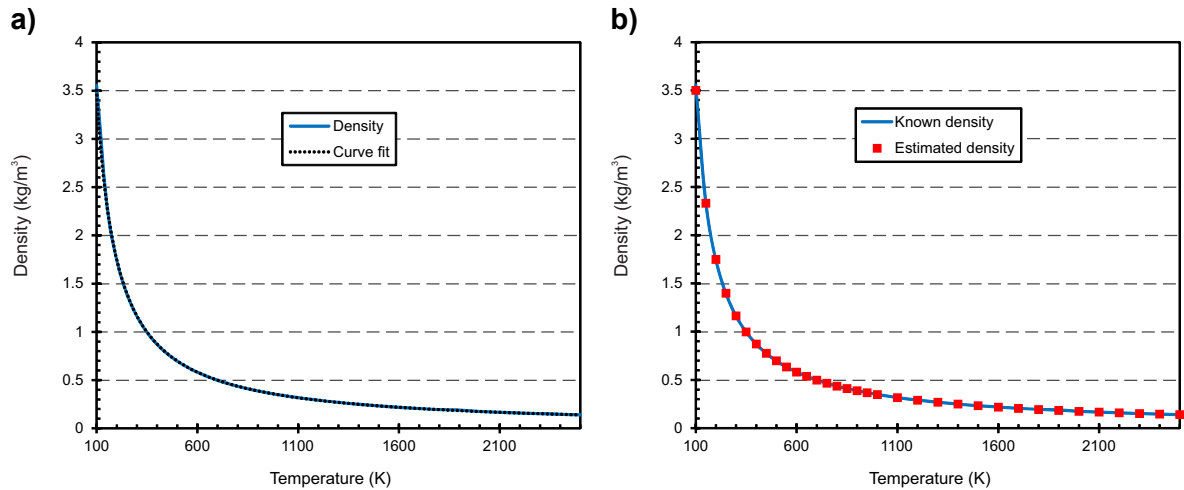


Figure C.1: a) curve fit to known density data and b) the comparison between the known data and estimated data using the determined equation.

The density of drying air values tabulated in Table C.1 are used to do a curve fitting as shown in Figure C.1 (a). From this the temperature dependent equation, that can be used to calculate the density of drying air at various air temperatures, is determined, i.e. Equation C.1. As can be seen from Figure C.1 (b), the determined equation is very accurate in estimating the density of drying air at various air temperatures.

$$\rho_g = 353.34 \times T_g^{-1.002} \quad \text{Equation C.1}$$

Equation C.1 is then implemented in Simulink®, as shown in Figure C.2, and used during the modelling of the roasting process.

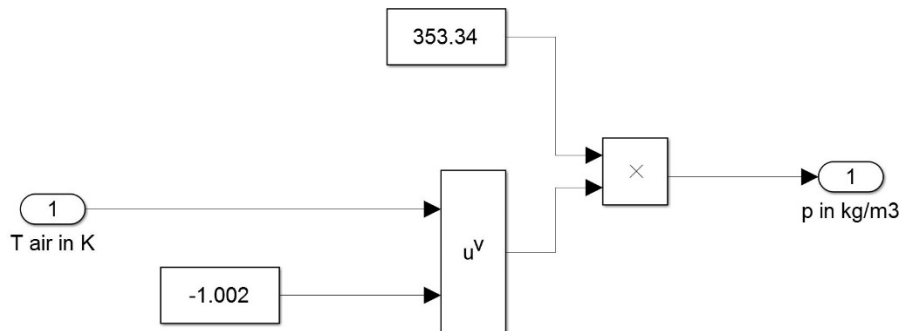


Figure C.2: Implementation of density in Simulink®.

C.2 Heat capacity of drying air

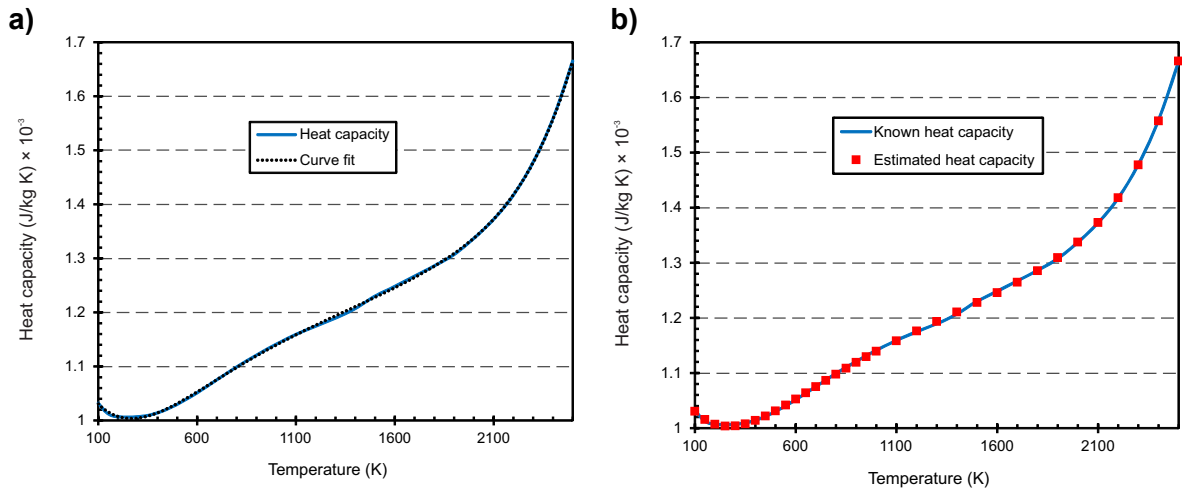


Figure C.3: a) curve fit to known heat capacity data and b) the comparison between the known data and estimated data using the determined equation.

The heat capacity of drying air values tabulated in Table C.1 are used to do a curve fitting as shown in Figure C.3 (a). From this the temperature dependent equation, that can be used to calculate the heat capacity of drying air at various air temperatures, is determined, i.e. Equation C.2. As can be seen from Figure C.3 (b), the determined equation is very accurate in estimating the heat capacity of drying air at various air temperatures.

$$\begin{aligned}
 c_{p_g} = & 5.3091 \times 10^{-17} [T_g^6] - 4.1550 \times 10^{-13} [T_g^5] + 1.3621 \times 10^{-9} [T_g^4] \\
 & - 2.3267 \times 10^{-6} [T_g^3] + 2.1034 \times 10^{-3} [T_g^2] \\
 & - 7.2075 \times 10^{-1} [T_g] + 1.0839 \times 10^+3
 \end{aligned}
 \tag{Equation C.2}$$

Equation C.2 is then implemented in Simulink®, as shown in Figure C.4, and used during the modelling of the roasting process.

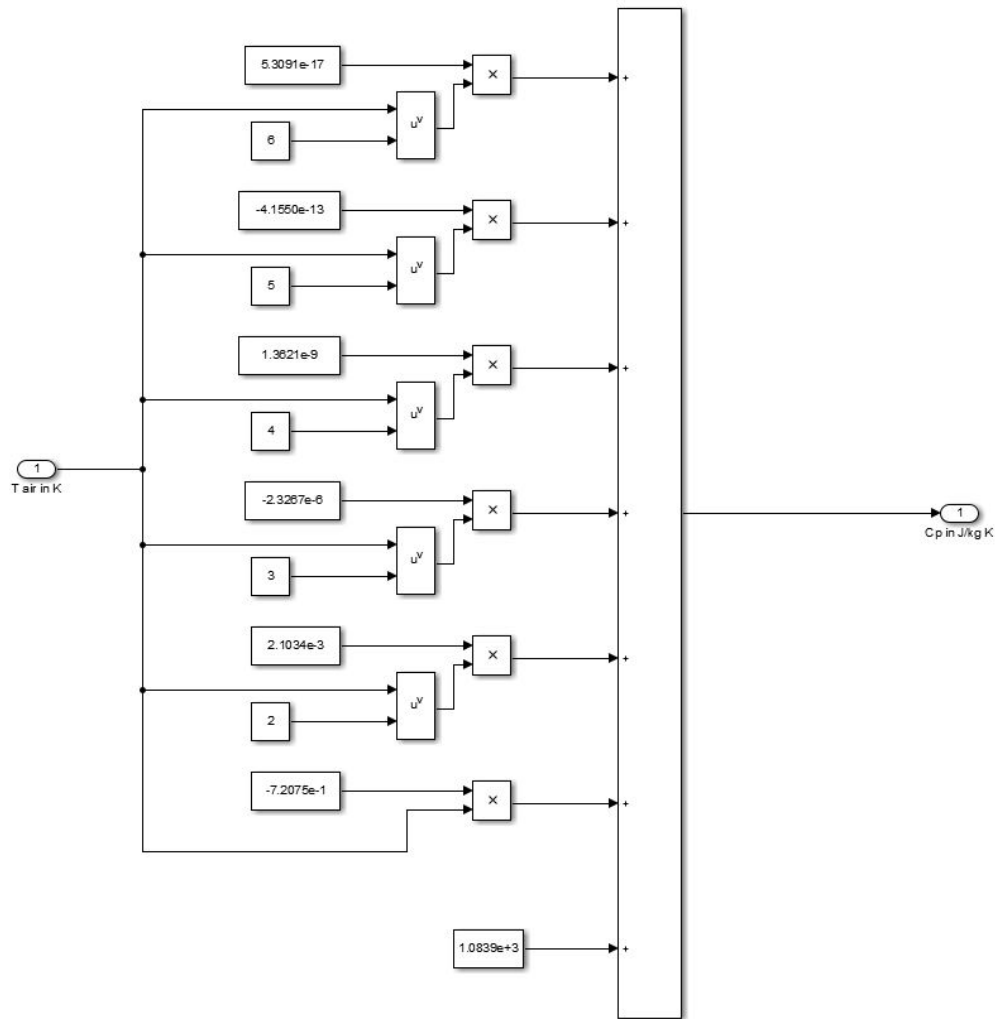


Figure C.4: Implementation of heat capacity in Simulink®.

C.3 Viscosity of drying air

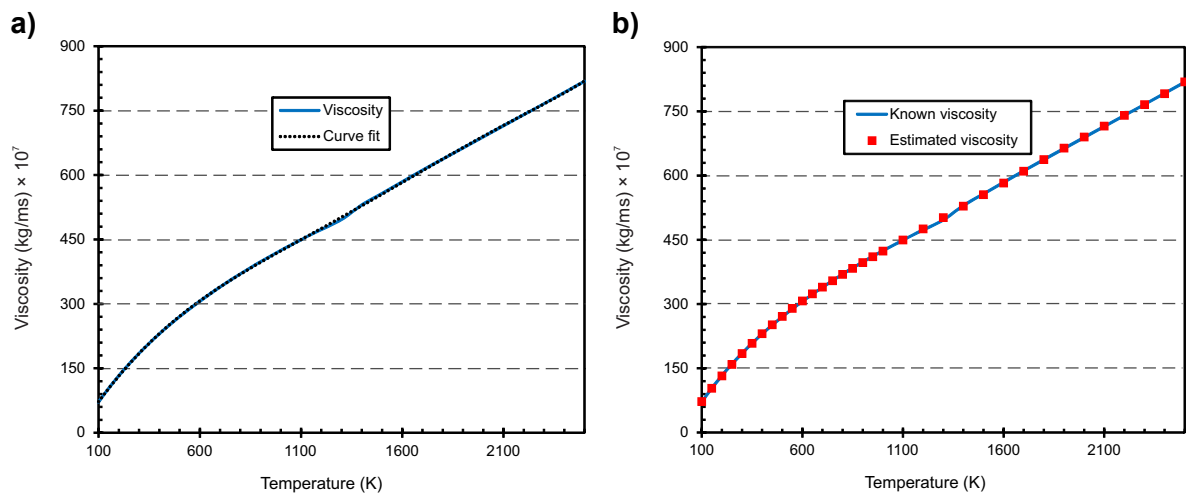


Figure C.5: a) curve fit to known viscosity data and b) the comparison between the known data and estimated data using the determined equation.

The viscosity of drying air values tabulated in Table C.1 are used to do a curve fitting as shown in Figure C.5 (a). From this the temperature dependent equation, that can be used to calculate the viscosity of drying air at various air temperatures, is determined, i.e. Equation C.3. As can be seen from Figure C.5 (b), the determined equation is very accurate in estimating the viscosity of drying air at various air temperatures.

$$\begin{aligned} \mu_g = & 1.2184 \times 10^{-24} [T_g^6] - 8.1123 \times 10^{-21} [T_g^5] + 1.6089 \times 10^{-17} [T_g^4] \\ & + 1.1460 \times 10^{-15} [T_g^3] - 3.9733 \times 10^{-11} [T_g^2] \\ & + 7.1226 \times 10^{-8} [T_g] + 4.8855 \times 10^{-7} \end{aligned} \quad \text{Equation C.3}$$

Equation C.3 is then implemented in Simulink®, as shown in Figure C.6, and used during the modelling of the roasting process.

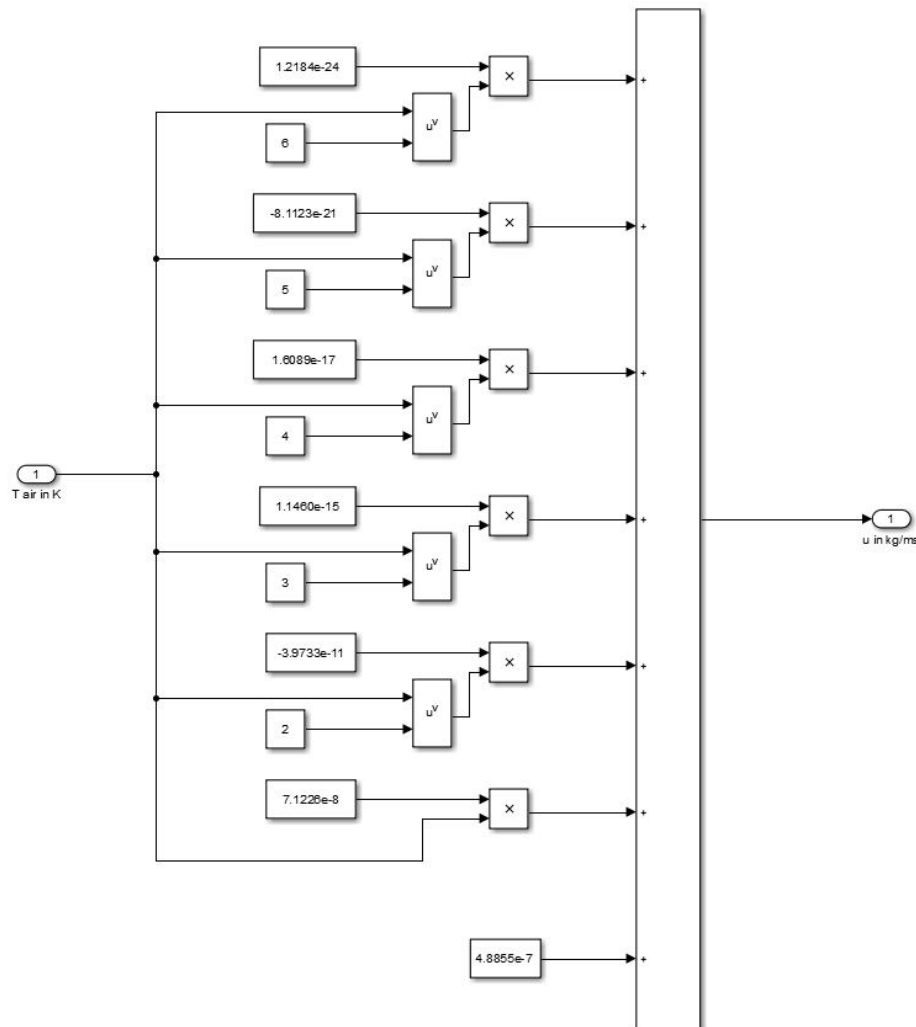


Figure C.6: Implementation of viscosity in Simulink®.

C.4 Thermal conductivity of drying air

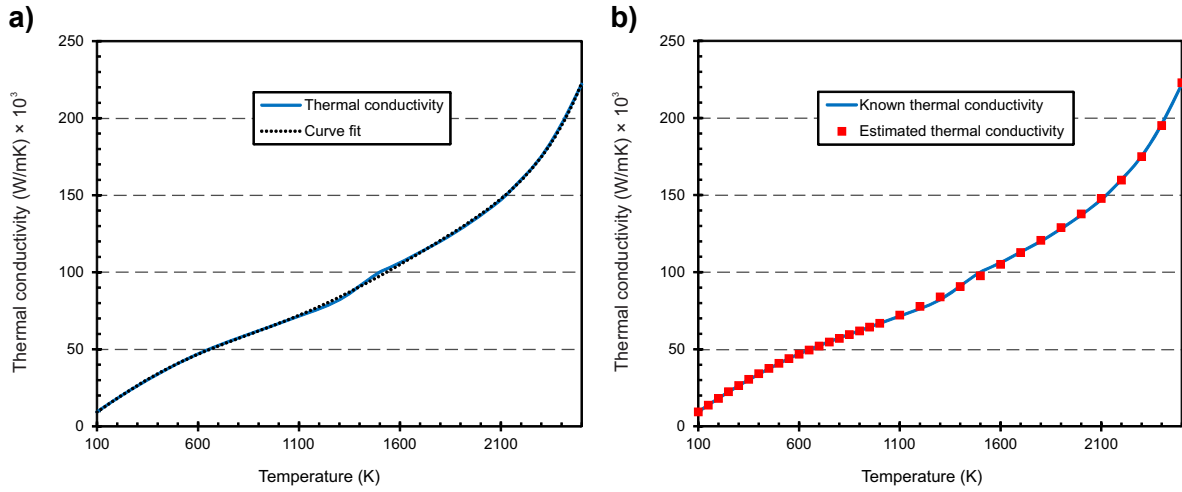


Figure C.7: a) curve fit to known thermal conductivity data and b) the comparison between the known data and estimated data using the determined equation.

The thermal conductivity of drying air values tabulated in Table C.1 are used to do a curve fitting as shown in Figure C.7 (a). From this the temperature dependent equation, that can be used to calculate the thermal conductivity of drying air at various air temperatures, is determined, i.e. Equation C.4. As can be seen from Figure C.7 (b), the determined equation is very accurate in estimating the thermal conductivity of drying air at various air temperatures.

$$\begin{aligned} \lambda_g = & 1.3819 \times 10^{-20} [T_g^6] - 9.1506 \times 10^{-17} [T_g^5] + 2.2342 \times 10^{-13} [T_g^4] \\ & - 2.2872 \times 10^{-10} [T_g^3] + 6.8867 \times 10^{-8} [T_g^2] \\ & + 8.0128 \times 10^{-5} [T_g] + 7.6694 \times 10^{-4} \end{aligned} \quad \text{Equation C.4}$$

Equation C.4 is then implemented in Simulink®, as shown in Figure C.8, and used during the modelling of the roasting process.

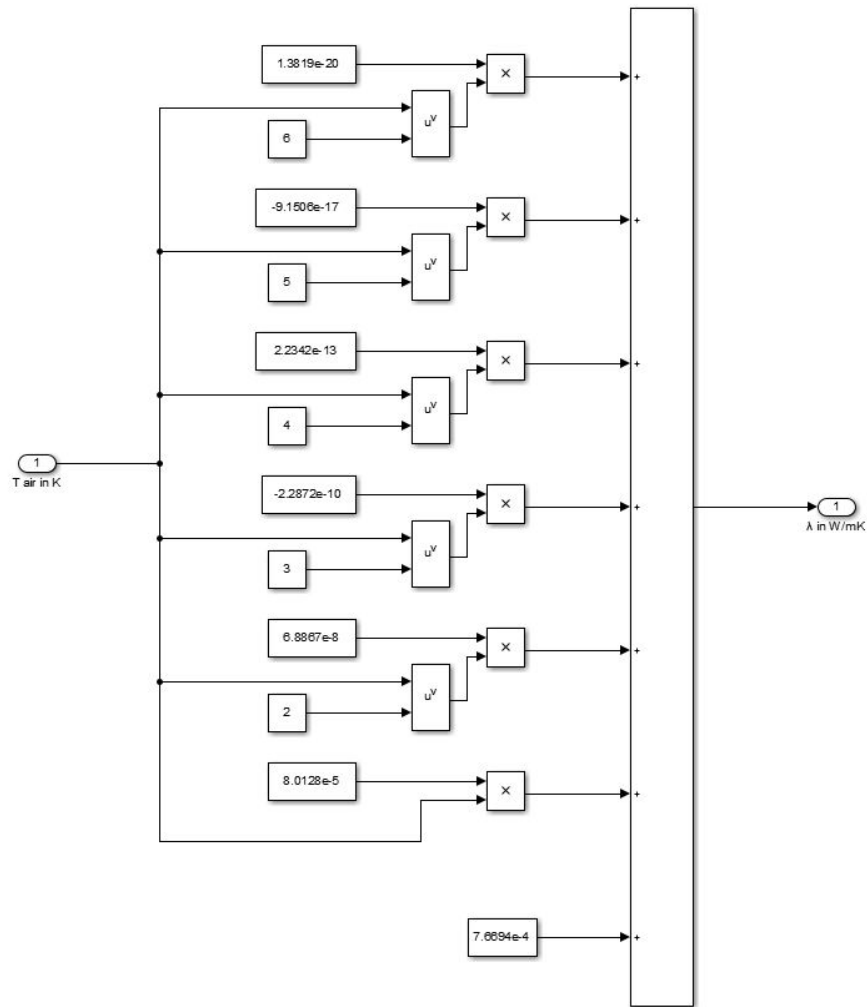


Figure C.8: Implementation of density in Simulink®.

Appendix D – Literature data used during calculations

Table D.1: Fabbri *et al.* (2011) experimental results used during heat capacity and thermal conductivity of coffee beans estimation.

Bean temperature	Time	Moisture content	
		mol/m ³	kg/kg
°C	s		
33.5	0	5380	0.152
169	120	4509	0.128
192	240	3478	0.099
203	360	2245	0.064
199	480	1603	0.045
200	600	977	0.028
200	840	426	0.012

Appendix E – Simulink models

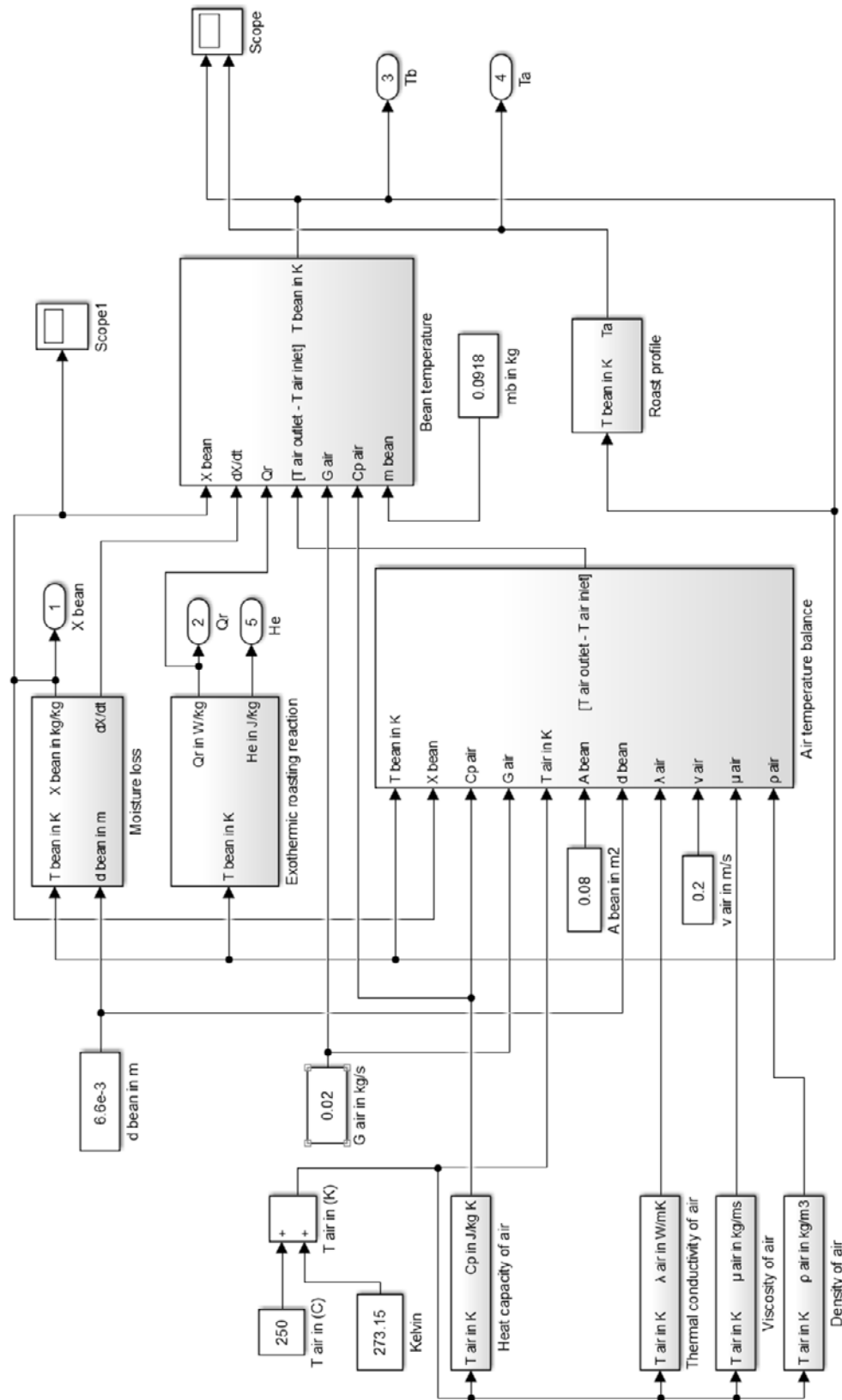


Figure E.1: Schwartzberg (2002) model implementation in Simulink®.

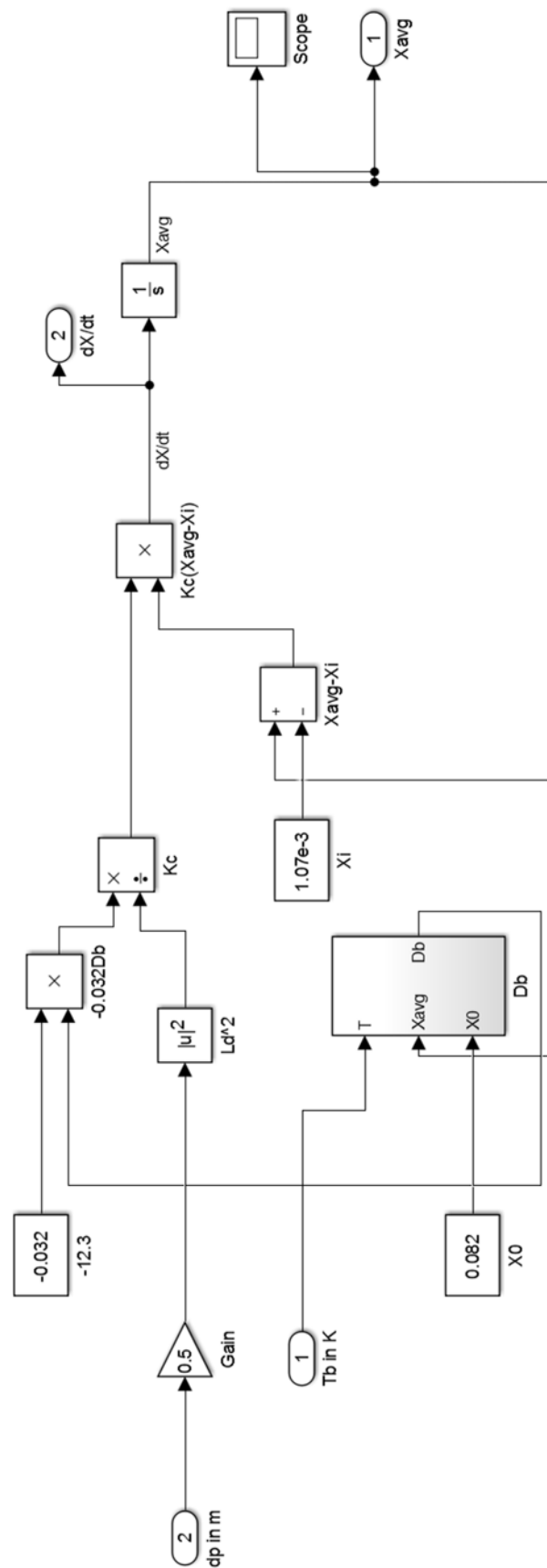


Figure E.2: Hernandez-Diaz et al. (2008) moisture model implementation in Simulink®.

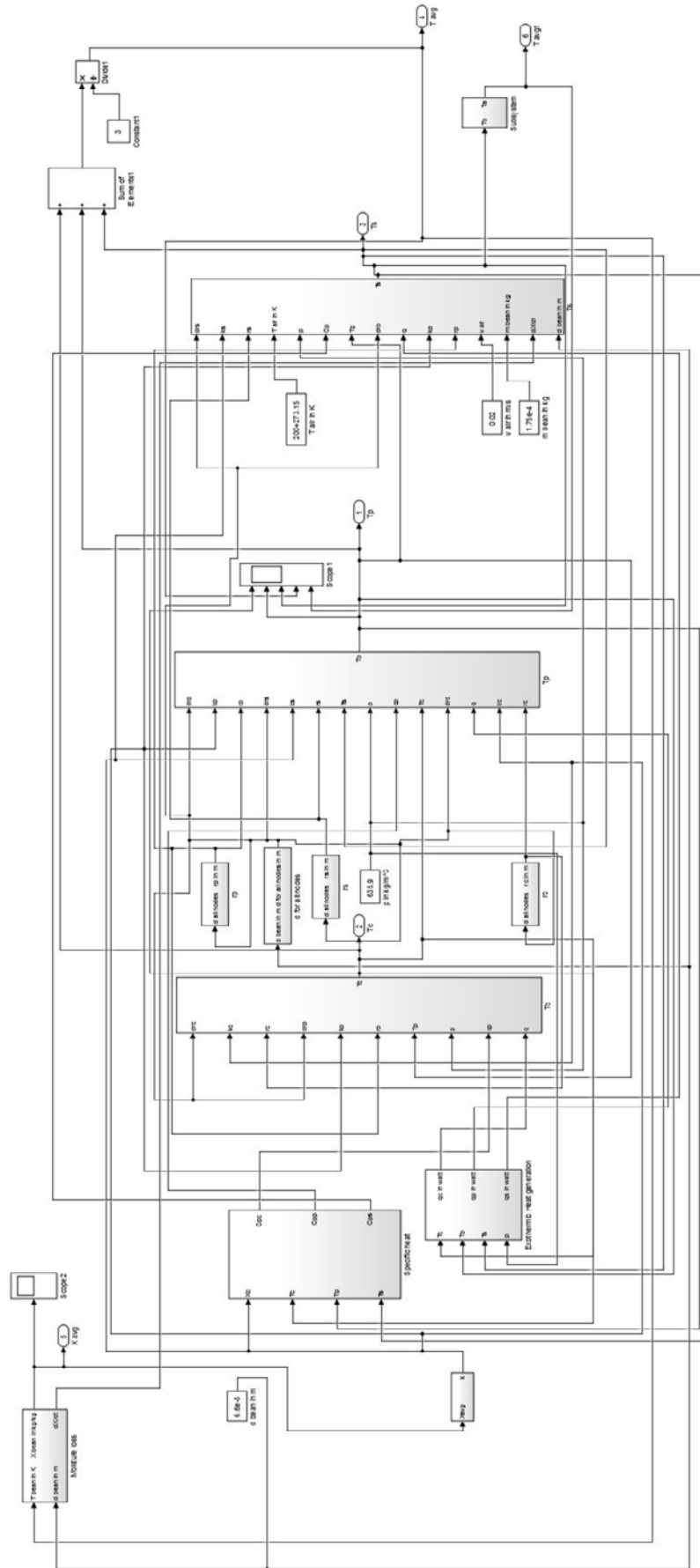


Figure E.4: Finite volume heat transfer model implementation in Simulink®.

Appendix F – Model parameters

F.1 Schwartzberg (2002) roast profile constant determination

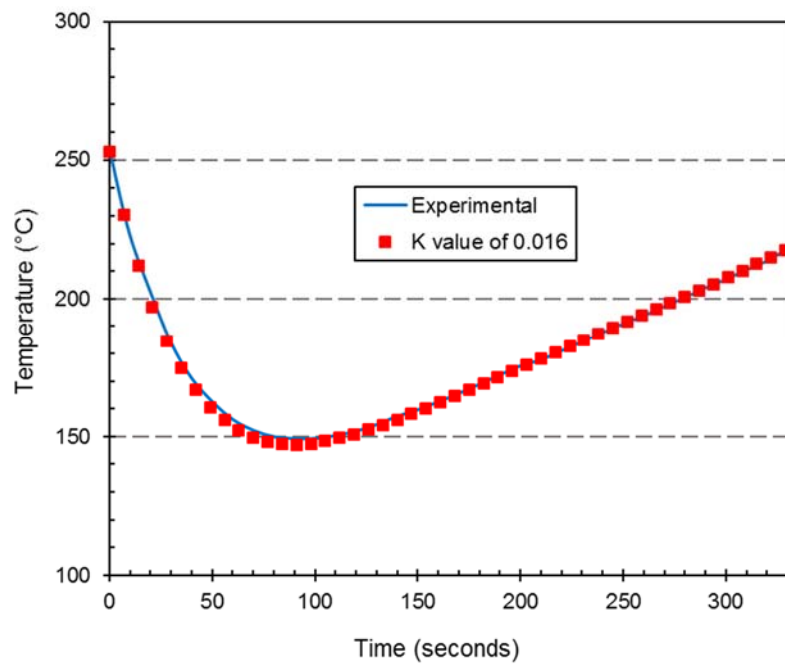


Figure F.1: Determination of roast profile constant from experimental results of Schwartzberg (2002).

F.2 Humidity influence on Putranto & Chen (2012) model

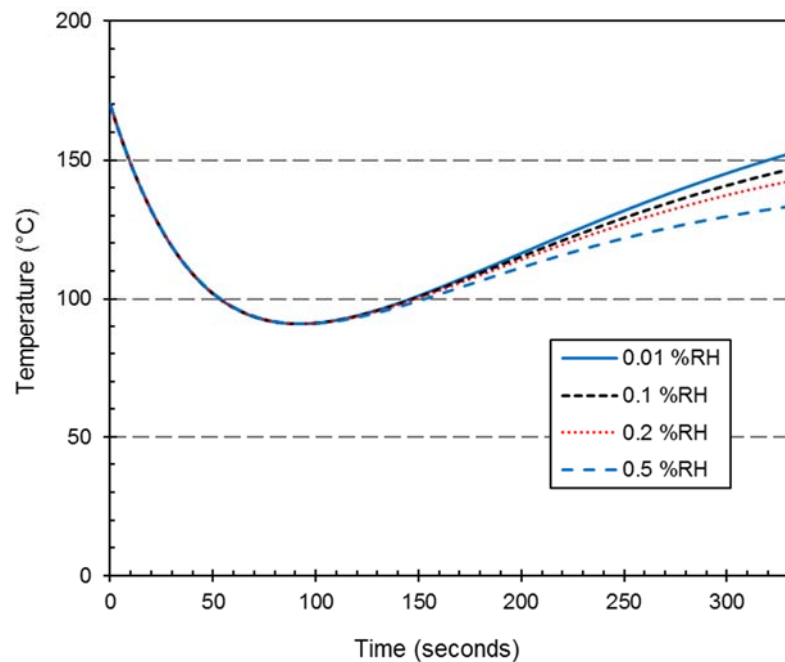


Figure F.2: Influence of inlet air relative humidity on the roast profile predicted with the Put_TX model

Appendix G – Roasting data

G.1 Roasting data for 10 minutes roast at various temperatures

G.1.1 170 °C

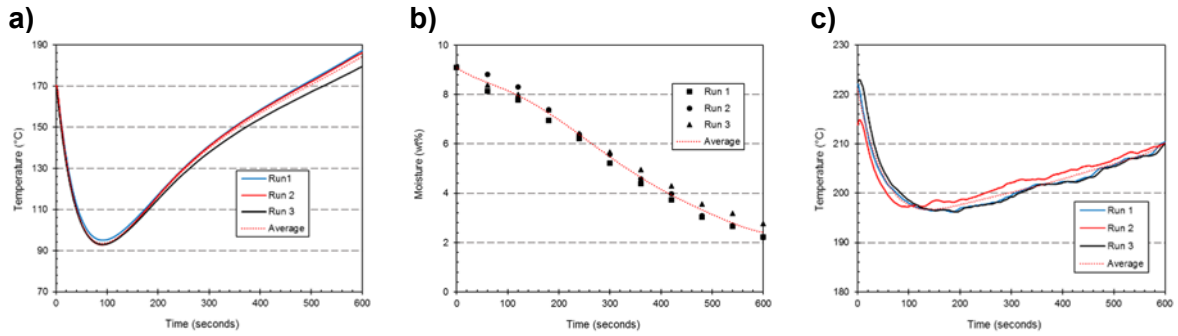


Figure G.1: Roasting data for 170 °C, a) roast profile, b) moisture content and c) air temperature.

Table G.1: Roast properties at 170 °C roast start.

Roast run	Batch weight		Roast loss (%)	Final moisture content (wt%)	Roast end temp (°C)
	Before (kg)	After (kg)			
Run 1	3.96	3.37	15.05	2.23	187
Run 2	3.84	3.42	10.97	2.21	186
Run 3	3.94	3.42	13.25	2.77	180

Table G.2: Temperature and time of when cracks occur at 170 °C roast start.

Roast run	Start first crack	
	Temp (°C)	Time (s)
Run 1	183	574
Run 2	177	535
Run 3	176	573

G.1.2 180 °C

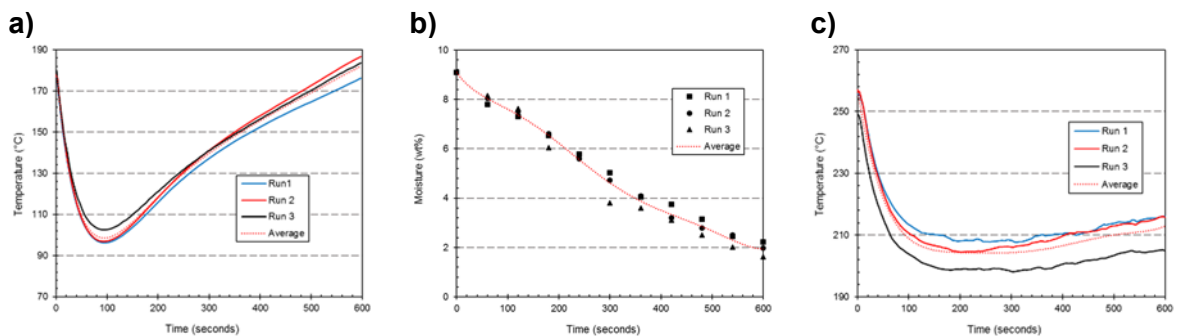


Figure G.2: Roasting data for 180 °C, a) roast profile, b) moisture content and c) air temperature.

Table G.3: Roast properties at 180 °C roast start.

Roast run	Batch weight		Roast loss (%)	Final moisture content (wt%)	Roast end temp (°C)
	Before (kg)	After (kg)			
Run 1	3.94	3.37	14.43	2.22	177
Run 2	3.92	3.41	13.09	1.97	187
Run 3	3.94	3.39	13.91	1.62	184

Table G.4: Temperature and time of when cracks occur at 180 °C roast start.

Roast run	Start first crack	
	Temp (°C)	Time (s)
Run 1	175	590
Run 2	177	527
Run 3	173	515

G.1.3 190 °C

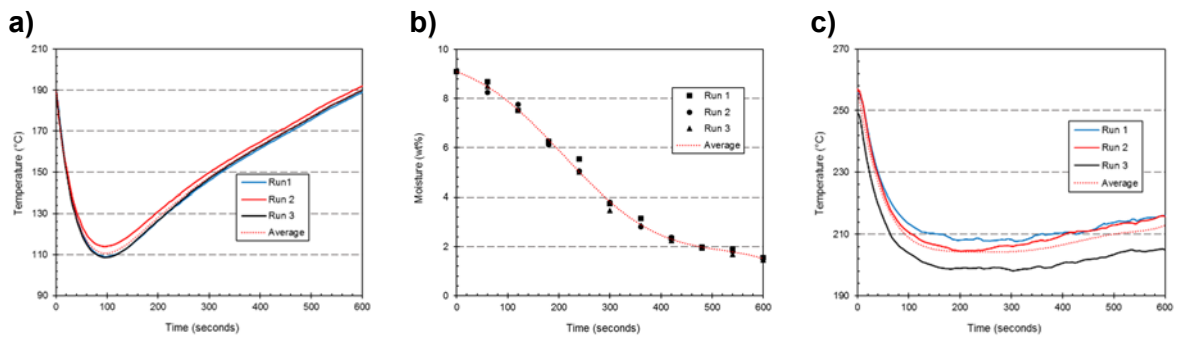


Figure G.3: Roasting data for 190 °C, a) roast profile, b) moisture content and c) air temperature.

Table G.5: Roast properties at 190 °C roast start.

Roast run	Batch weight		Roast loss (%)	Final moisture content (wt%)	Roast end temp (°C)
	Before (kg)	After (kg)			
Run 1	3.92	3.34	14.72	1.54	189
Run 2	3.95	3.38	14.44	1.55	192
Run 3	3.93	3.33	15.43	1.45	190

Table G.6: Temperature and time of when cracks occur at 190 °C roast start.

Roast run	Start first crack		End first crack	
	Temp (°C)	Time (s)	Temp (°C)	Time (s)
Run 1	175	495	-	-
Run 2	176	475	189	575
Run 3	175	485	188	585

G.1.4 200 °C

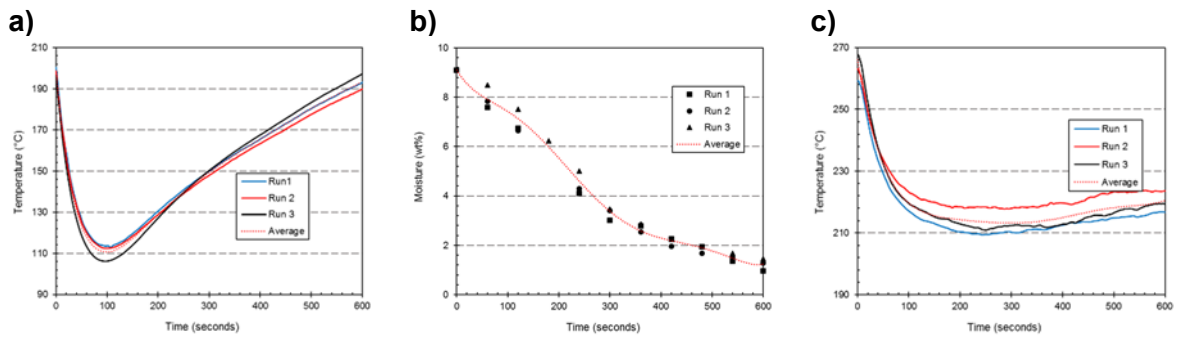


Figure G.4: Roasting data for 200 °C, a) roast profile, b) moisture content and c) air temperature.

Table G.7: Roast properties at 200 °C roast start.

Roast run	Batch weight		Roast loss (%)	Final moisture content (wt%)	Roast end temp (°C)
	Before (kg)	After (kg)			
Run 1	3.96	3.33	15.80	0.96	193
Run 2	3.95	3.33	15.53	1.27	190
Run 3	3.93	3.37	14.15	1.45	197

Table G.8: Temperature and time of when cracks occur at 200 °C roast start.

Roast run	Start first crack		End first crack	
	Temp (°C)	Time (s)	Temp (°C)	Time (s)
Run 1	173	450	190	570
Run 2	174	475	190	595
Run 3	176	485	-	-

G.1.5 210 °C

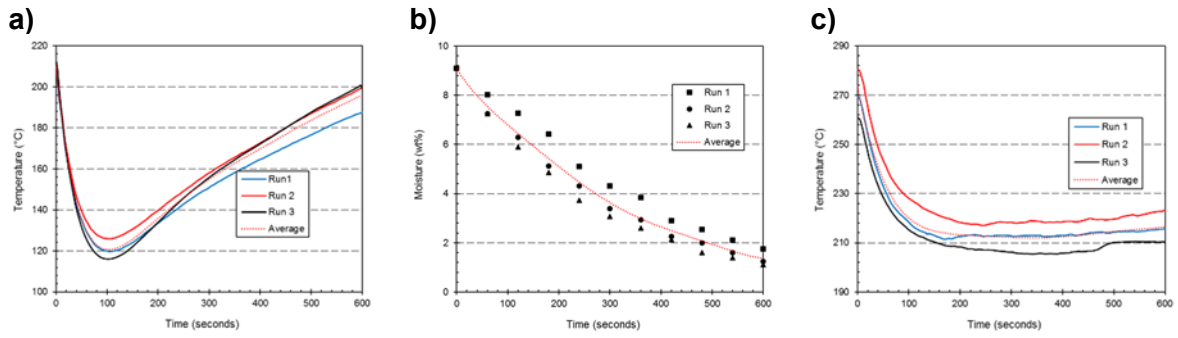


Figure G.5: Roasting data for 210 °C, a) roast profile, b) moisture content and c) air temperature.

Table G.9: Roast properties at 210 °C roast start.

Roast run	Batch weight		Roast loss (%)	Final moisture content (wt%)	Roast end temp (°C)
	Before (kg)	After (kg)			
Run 1	3.93	3.36	14.58	1.74	188
Run 2	3.93	3.36	14.48	1.24	200
Run 3	3.95	3.34	16.00	1.11	197

Table G.10: Temperature and time of when cracks occur at 210 °C roast start.

Roast run	Start first crack		End first crack	
	Temp (°C)	Time (s)	Temp (°C)	Time (s)
Run 1	171	436	185	600
Run 2	184	491	-	-
Run 3	176	435	192	537

G.1.6 220 °C

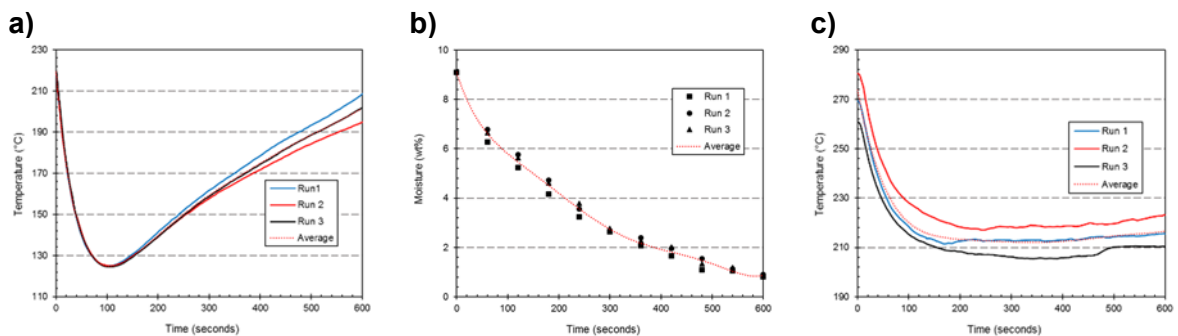


Figure G.6: Roasting data for 220 °C, a) roast profile, b) moisture content and c) air temperature.

Table G.11: Roast properties at 220 °C roast start.

Roast run	Batch weight		Roast loss (%)	Final moisture content (wt%)	Roast end temp (°C)
	Before (kg)	After (kg)			
Run 1	3.82	3.13	18.04	0.81	209
Run 2	3.81	3.27	14.34	0.92	195
Run 3	3.95	3.32	16.04	0.87	202

Table G.12: Temperature and time of when cracks occur at 220 °C roast start.

Roast run	Start first crack		End first crack		Start second crack	
	Temp (°C)	Time (s)	Temp (°C)	Time (s)	Temp (°C)	Time (s)
Run 1	177	384	196	514	202	560
Run 2	179	450	191	562	-	-
Run 3	176	412	193	535	199	580

G.1.7 230 °C

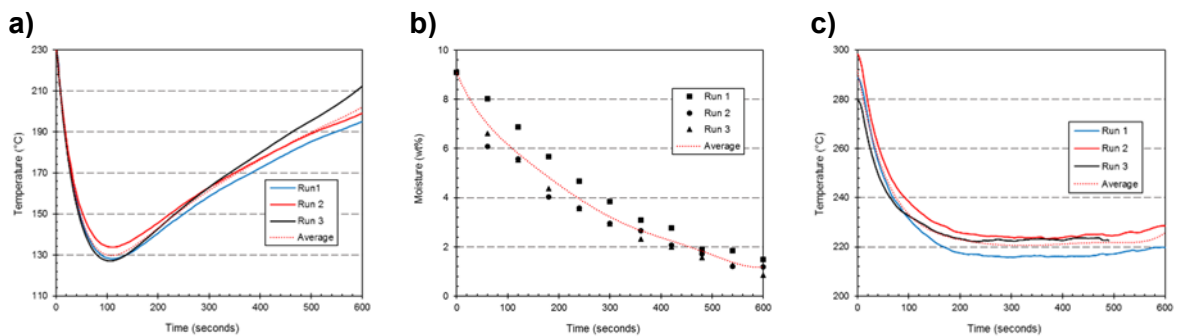


Figure G.7: Roasting data for 230 °C, a) roast profile, b) moisture content and c) air temperature.

Table G.13: Roast properties at 230 °C roast start.

Roast run	Batch weight		Roast loss (%)	Final moisture content (wt%)	Roast end temp (°C)
	Before (kg)	After (kg)			
Run 1	3.93	3.25	17.43	1.49	195
Run 2	3.95	3.38	14.51	1.19	199
Run 3	3.90	3.33	14.65	0.85	212

Table G.14: Temperature and time of when cracks occur at 230 °C roast start.

Roast run	Start first crack		End first crack		Start second crack	
	Temp (°C)	Time (s)	Temp (°C)	Time (s)	Temp (°C)	Time (s)
Run 1	181	384	186	515	203	550
Run 2	184	448	191	556	-	-
Run 3	179	412	193	535	197	585

G.1.8 240 °C

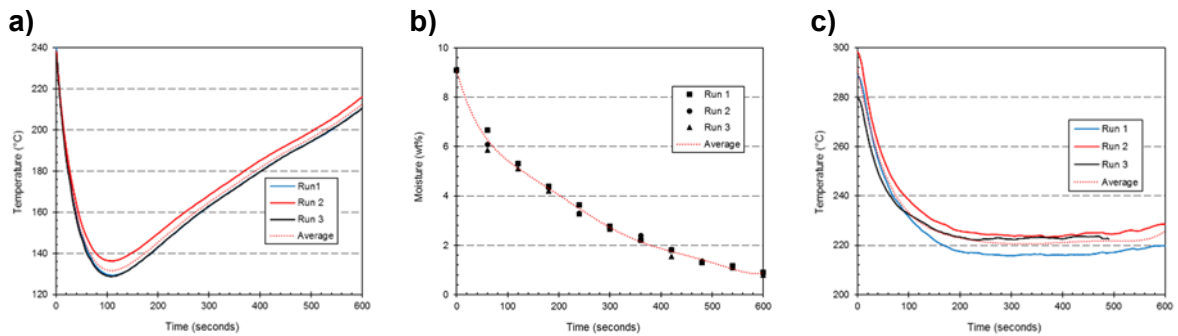


Figure G.8: Roasting data for 240 °C, a) roast profile, b) moisture content and c) air temperature.

Table G.15: Roast properties at 240 °C roast start.

Roast run	Batch weight		Roast loss (%)	Final moisture content (wt%)	Roast end temp (°C)
	Before (kg)	After (kg)			
Run 1	3.96	3.19	19.51	0.91	211
Run 2	3.92	3.10	20.81	0.86	216
Run 3	3.94	3.16	19.99	0.80	211

Table G.16: Temperature and time of when cracks occur at 240 °C roast start.

Roast run	Start first crack		End first crack		Start second crack	
	Temp (°C)	Time (s)	Temp (°C)	Time (s)	Temp (°C)	Time (s)
Run 1	175	369	194	491	200	535
Run 2	178	357	197	482	201	512
Run 3	176	376	200	496	203	525

G.2 Roasting data for roasting until second crack at various temperatures

G.2.1 170 °C

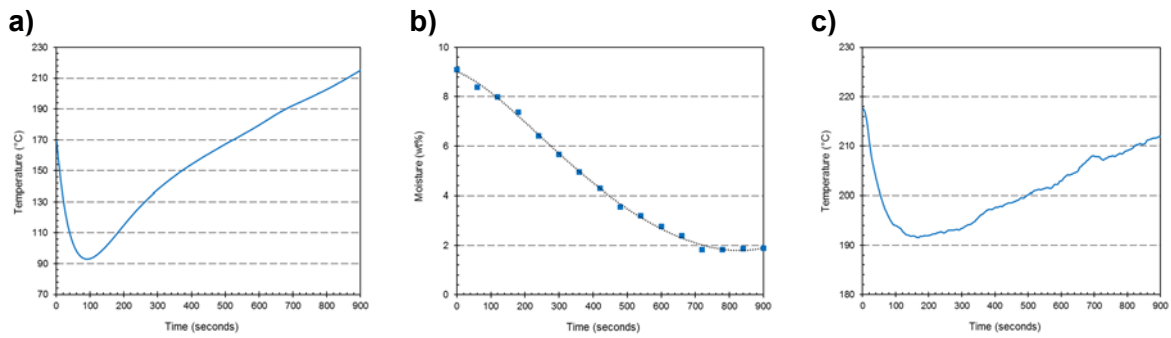


Figure G.9: Roasting data for 170 °C, a) roast profile, b) moisture content and c) air temperature.

G.2.2 180 °C

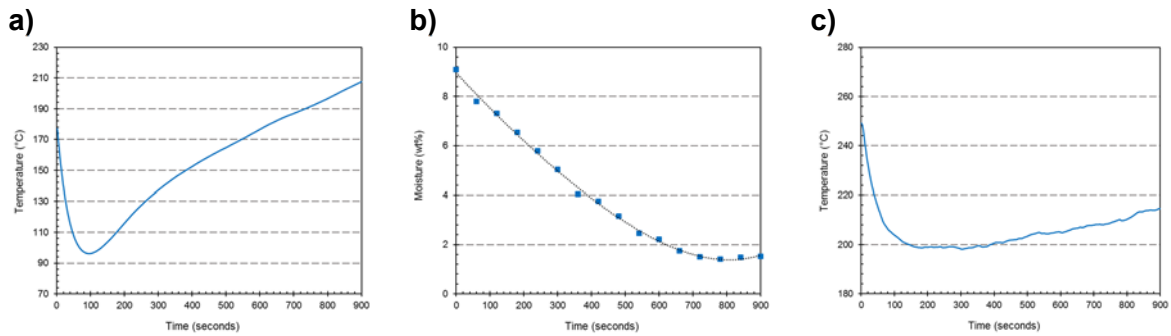


Figure G.10: Roasting data for 180 °C, a) roast profile, b) moisture content and c) air temperature.

G.2.3 190 °C

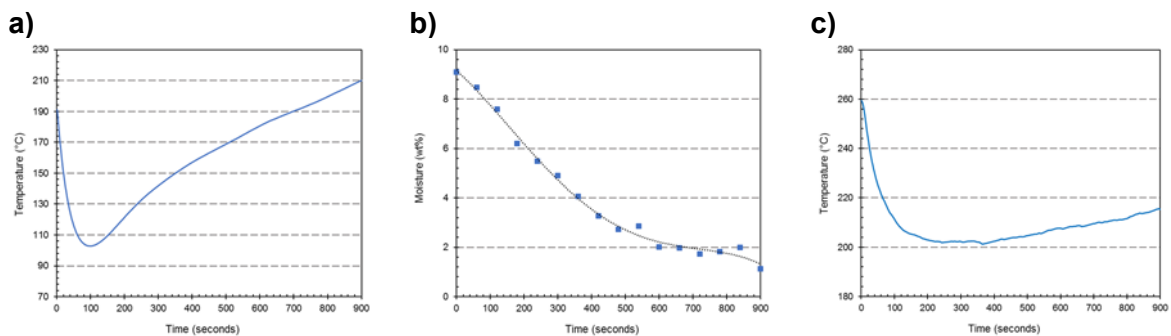


Figure G.11: Roasting data for 190 °C, a) roast profile, b) moisture content and c) air temperature.

G.2.4 200 °C

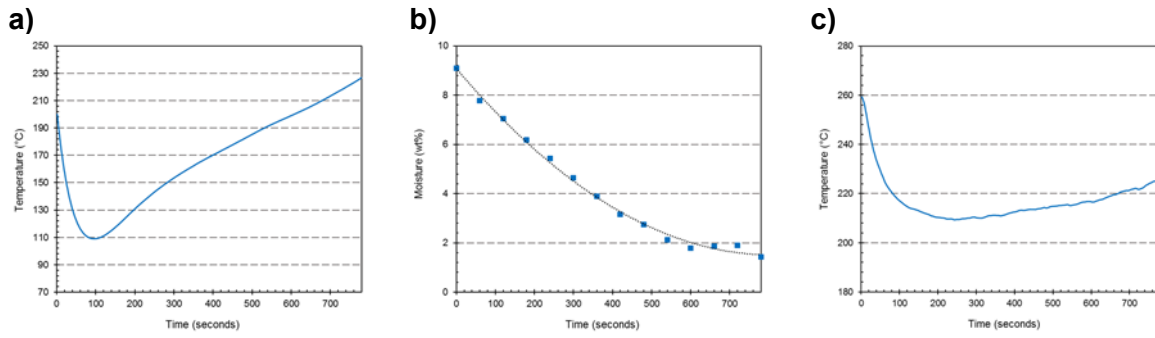


Figure G.12: Roasting data for 200 °C, a) roast profile, b) moisture content and c) air temperature.

G.2.5 210 °C

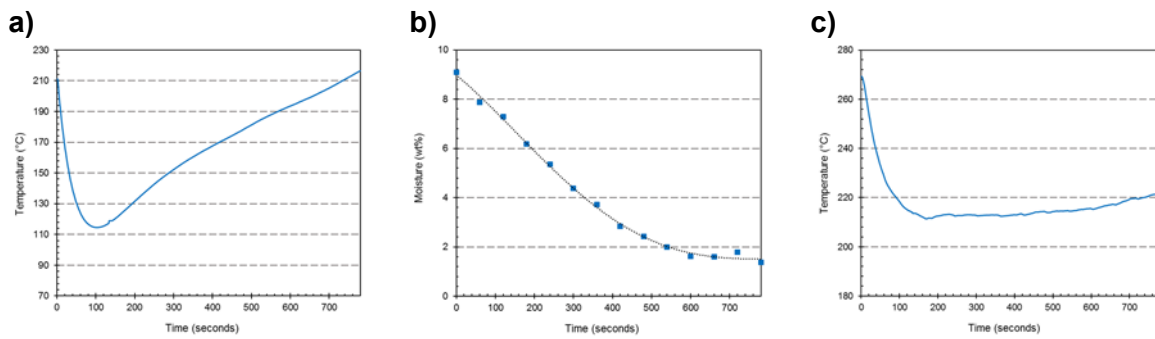


Figure G.13: Roasting data for 210 °C, a) roast profile, b) moisture content and c) air temperature.

G.2.6 220 °C

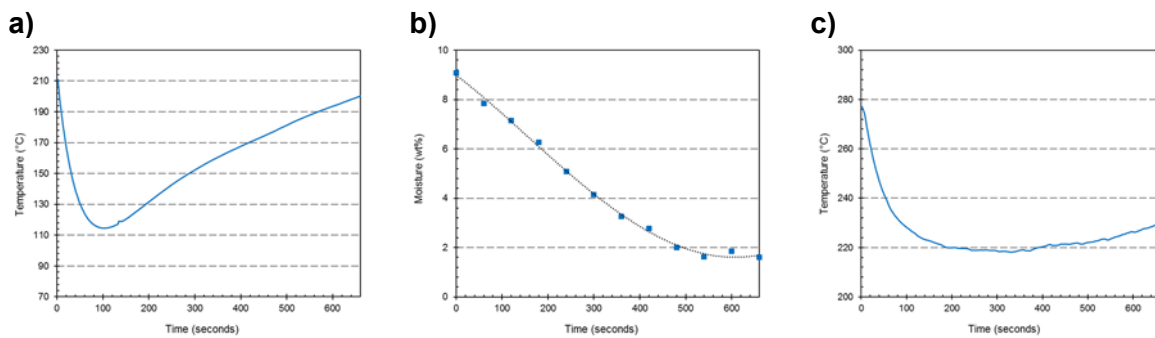


Figure G.14: Roasting data for 220 °C, a) roast profile, b) moisture content and c) air temperature.

G.2.7 230 °C

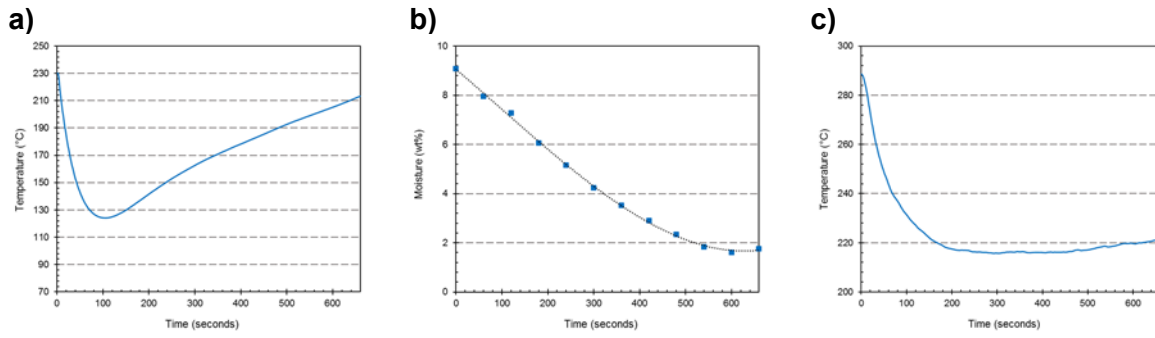


Figure G.15: Roasting data for 230 °C, a) roast profile, b) moisture content and c) air temperature.

G.2.8 240 °C

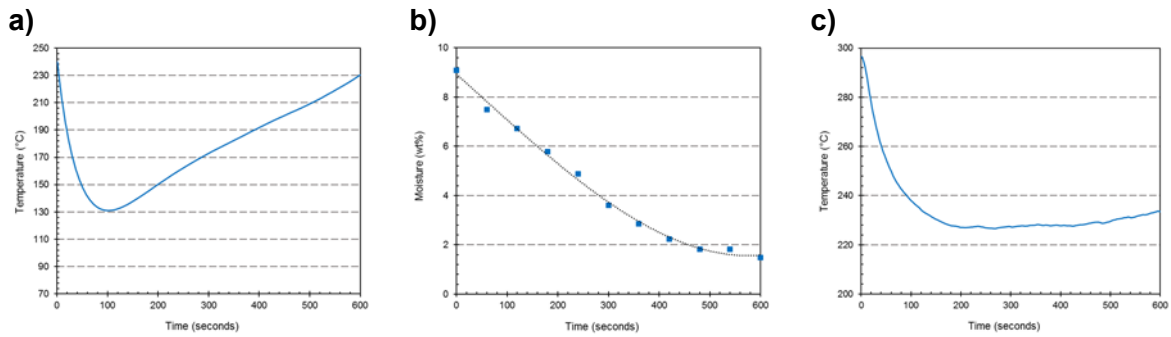


Figure G.16: Roasting data for 240 °C, a) roast profile, b) moisture content and c) air temperature.

G.3 Roasting data for roasting with increased moisture content

G.3.1 12.7 wt%

G.3.1.1 170 °C

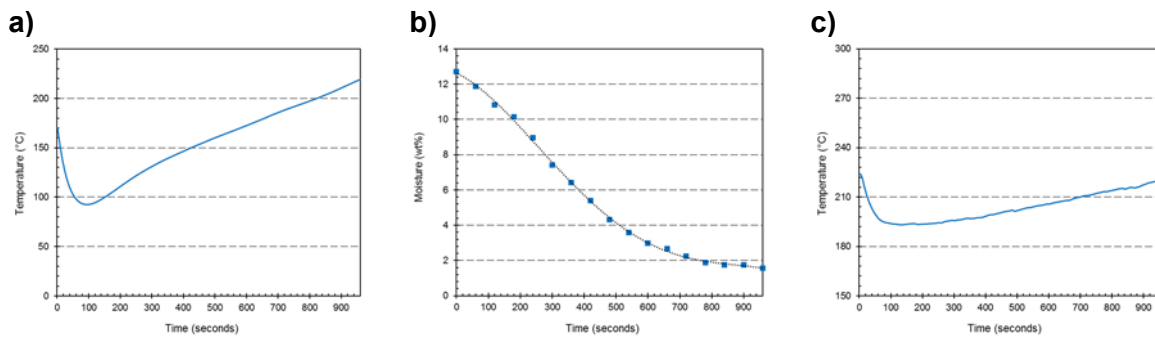


Figure G.17: Roasting data for 170 °C, a) roast profile, b) moisture content and c) air temperature.

G.3.1.2 190 °C

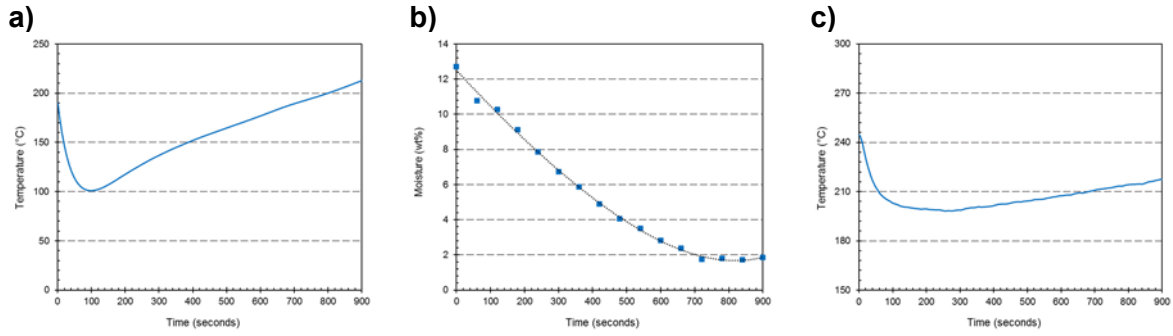


Figure G.18: Roasting data for 190 °C, a) roast profile, b) moisture content and c) air temperature.

G.3.1.3 210 °C

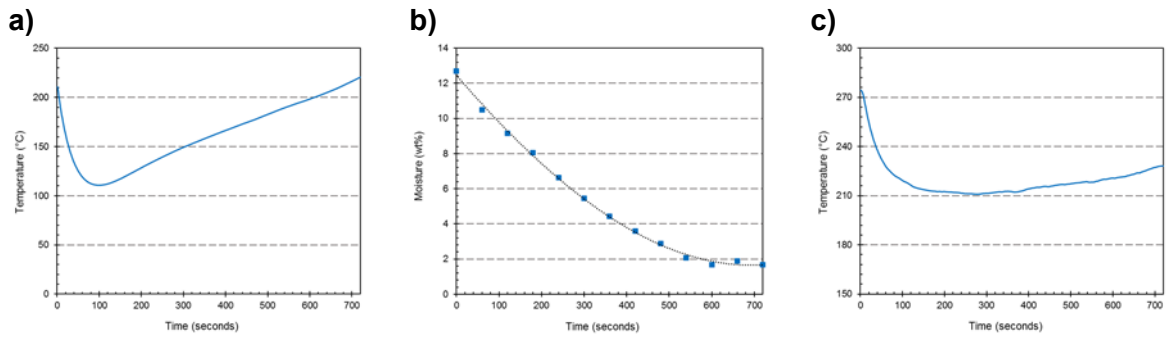


Figure G.19: Roasting data for 210 °C, a) roast profile, b) moisture content and c) air temperature.

G.3.1.4 230 °C

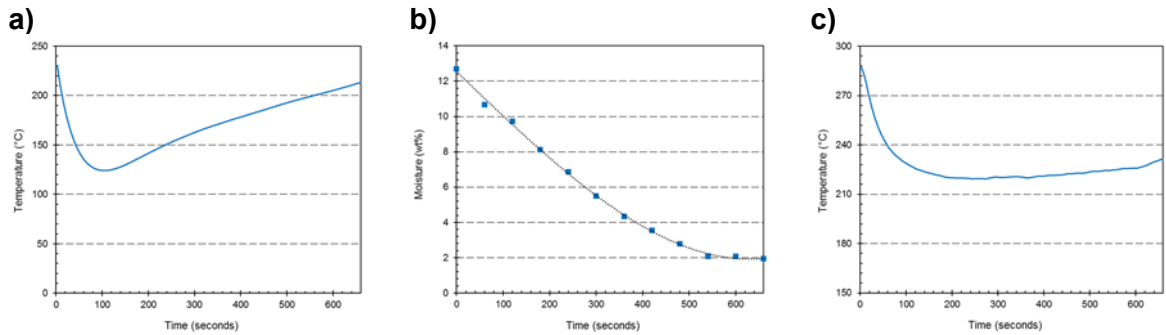


Figure G.20: Roasting data for 230 °C, a) roast profile, b) moisture content and c) air temperature.

Table G.17: Roasting properties determined for the various roast start temperatures, for roasts conducted with 12.7 wt% moisture content coffee beans.

Roast start temp (°C)	Roast loss (%)	Final moisture content (wt%)	Roast end temp (°C)	Roasting time (s)
170	22.4	1.56	219	960
190	19.9	1.85	213	900
210	22.7	1.67	221	720
230	21.5	1.93	219	660

Table G.18: Temperature and roasting time for when the first and second crack occurs, for roast conducted with 12.7 wt% moisture content coffee beans.

Roast start temp (°C)	Start first crack		End first crack		Start second crack	
	Temp (°C)	Time (s)	Temp (°C)	Time (s)	Temp (°C)	Time (s)
170	179	648	196	789	203	847
190	177	604	195	754	203	825
210	176	459	203	628	204	637
230	176	413	203	580	206	597

G.3.2 13.3 wt%

G.3.2.1 170 °C

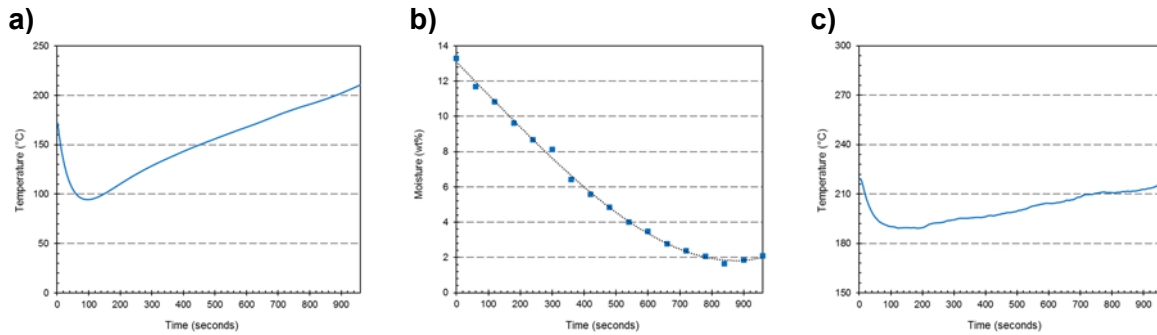


Figure G.21: Roasting data for 170 °C, a) roast profile, b) moisture content and c) air temperature.

G.3.2.2 190 °C

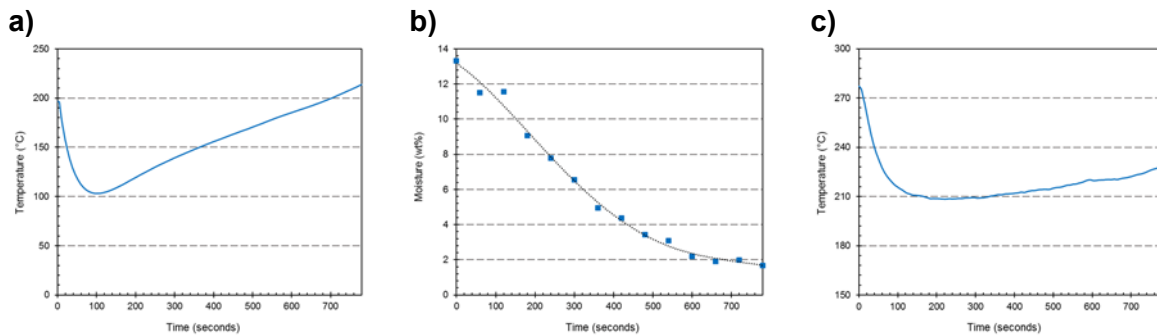


Figure G.22: Roasting data for 190 °C, a) roast profile, b) moisture content and c) air temperature.

G.3.2.3 210 °C

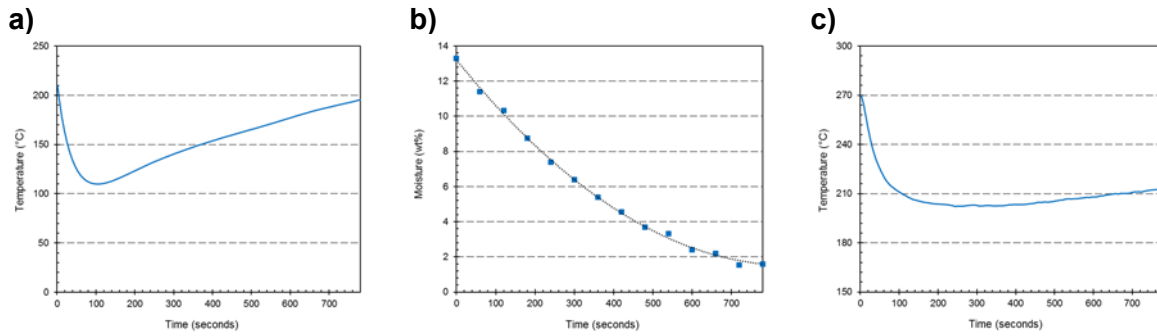


Figure G.23: Roasting data for 210 °C, a) roast profile, b) moisture content and c) air temperature.

G.3.2.4 230 °C

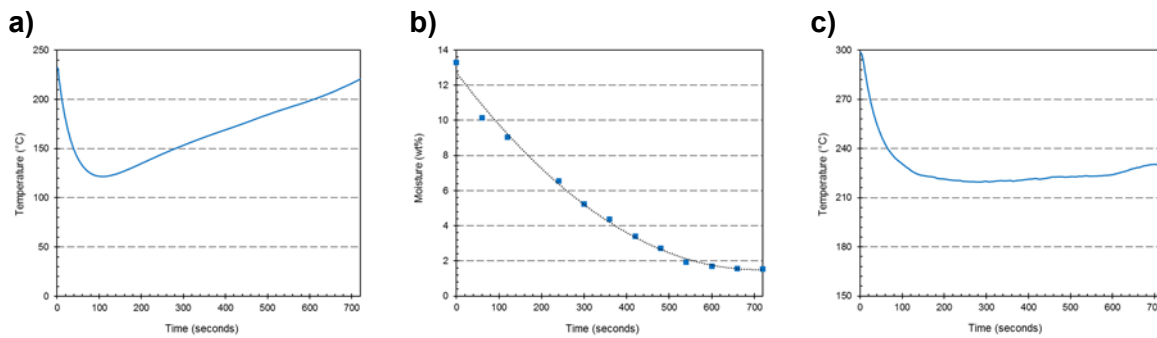


Figure G.24: Roasting data for 230 °C, a) roast profile, b) moisture content and c) air temperature.

Table G.19: Roasting properties determined for the various roast start temperatures, for roasts conducted with 13.3 wt% moisture content coffee beans.

Roast start temp (°C)	Roast loss (%)	Final moisture content (wt%)	Roast end temp (°C)	Roasting time (s)
170	21.0	2.09	211	960
190	21.4	1.67	214	780
210	20.5	1.81	209	780
230	24.2	1.55	221	720

Table G.20: Temperature and roasting time for when the first and second crack occurs, for roast conducted with 13.3 wt% moisture content coffee beans.

Roast start temp (°C)	Start first crack		End first crack		Start second crack	
	Temp (°C)	Time (s)	Temp (°C)	Time (s)	Temp (°C)	Time (s)
170	176	668	194	833	201	887
190	177	545	195	674	201	706
210	175	579	196	785	203	845
230	177	453	197	586	203	628

G.3.3 14.5 wt%

G.3.3.1 170 °C

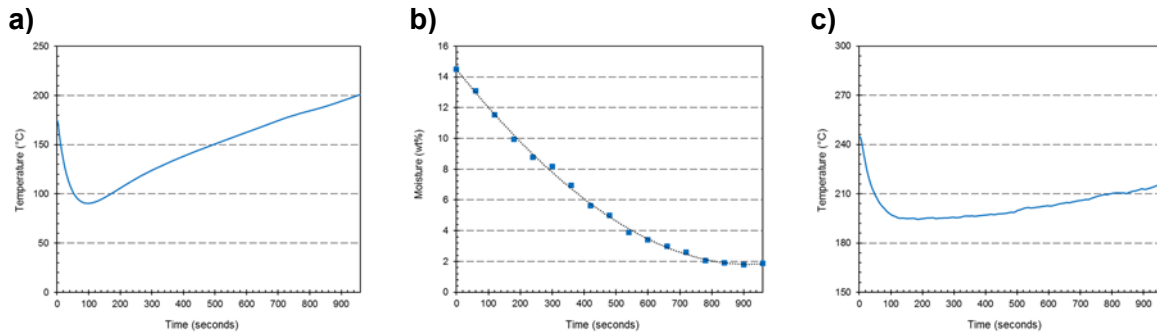


Figure G.25: Roasting data for 170 °C, a) roast profile, b) moisture content and c) air temperature.

G.3.3.2 190 °C

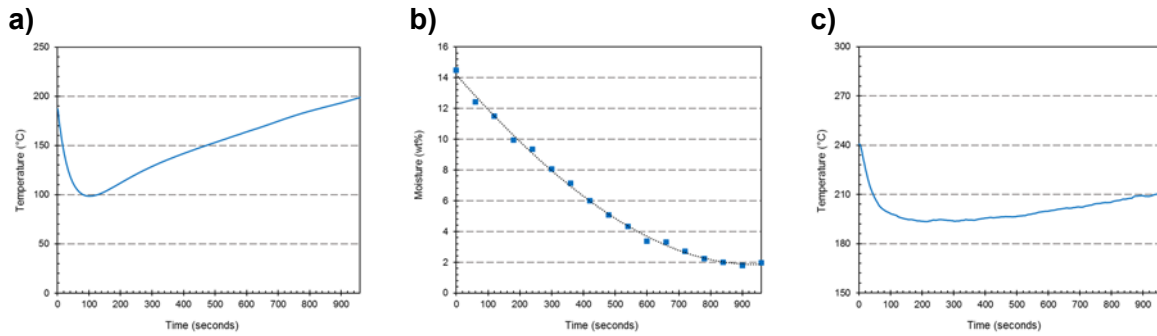


Figure G.26: Roasting data for 190 °C, a) roast profile, b) moisture content and c) air temperature.

G.3.3.3 210 °C

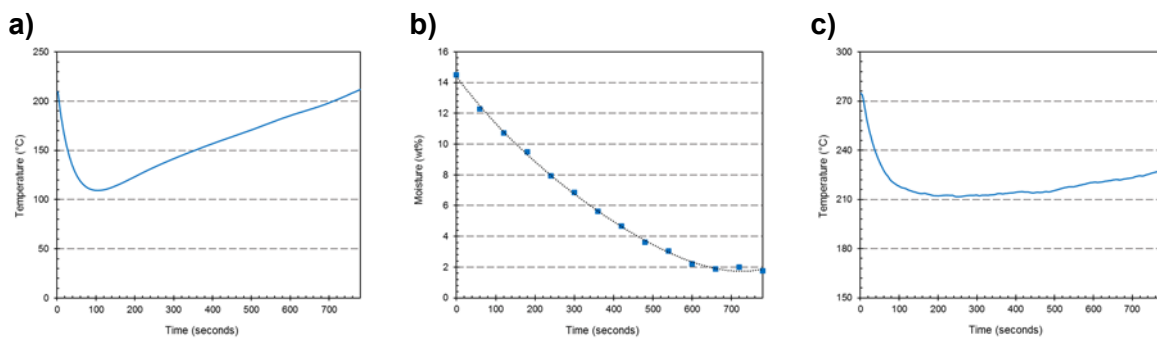


Figure G.27: Roasting data for 210 °C, a) roast profile, b) moisture content and c) air temperature.

G.3.3.4 230 °C

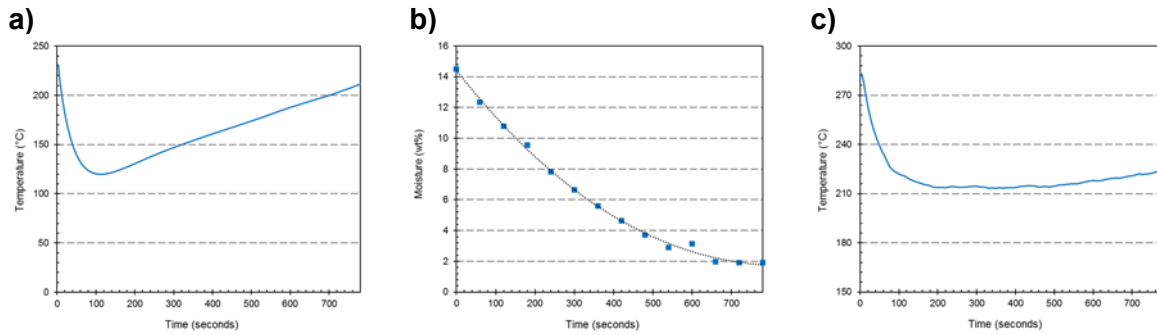


Figure G.28: Roasting data for 230 °C, a) roast profile, b) moisture content and c) air temperature.

Table G.21: Roasting properties determined for the various roast start temperatures, for roasts conducted with 14.5 wt% moisture content coffee beans.

Roast start temp (°C)	Roast loss (%)	Final moisture content (wt%)	Roast end temp (°C)	Roasting time (s)
170	20.9	1.89	201	960
190	21.5	1.95	199	960
210	23.1	1.75	212	780
230	25.2	1.65	211	780

Table G.22: Temperature and roasting time for when the first and second crack occurs, for roast conducted with 14.5 wt% moisture content coffee beans.

Roast start temp (°C)	Start first crack		End first crack		Start second crack	
	Temp (°C)	Time (s)	Temp (°C)	Time (s)	Temp (°C)	Time (s)
170	179	739	190	860	197	922
190	182	764	190	866	198	955
210	174	525	194	668	202	720
230	182	557	198	680	204	730

Appendix H – Modelling validation results

H.1 Put_TX results before adjustment

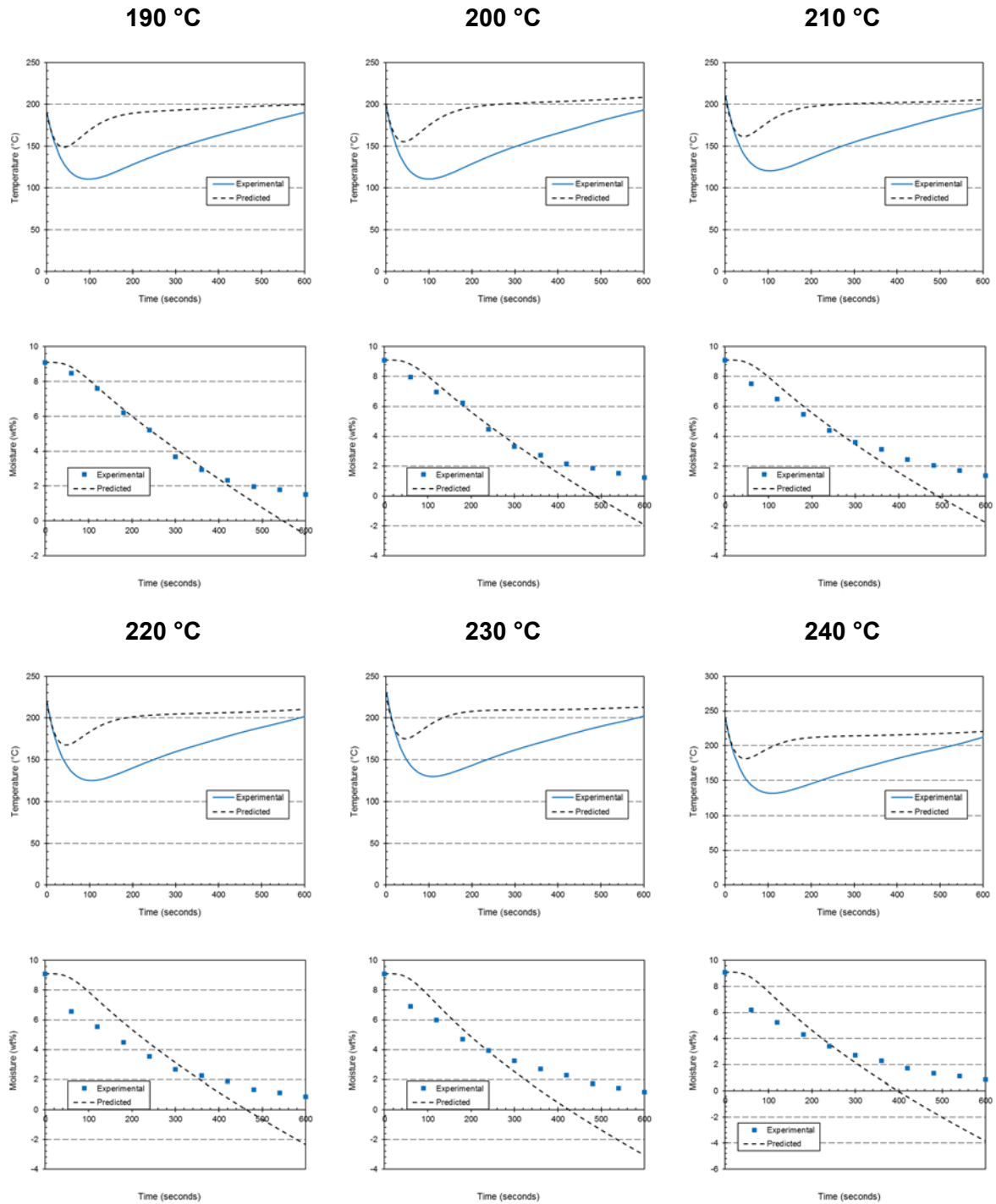


Figure H.1: Modelling validation results of Put_TX model before surface area adjustment, at higher roasting temperatures.

H.2 Validation results for 10 minutes roast at various temperatures

H.2.1 180 °C

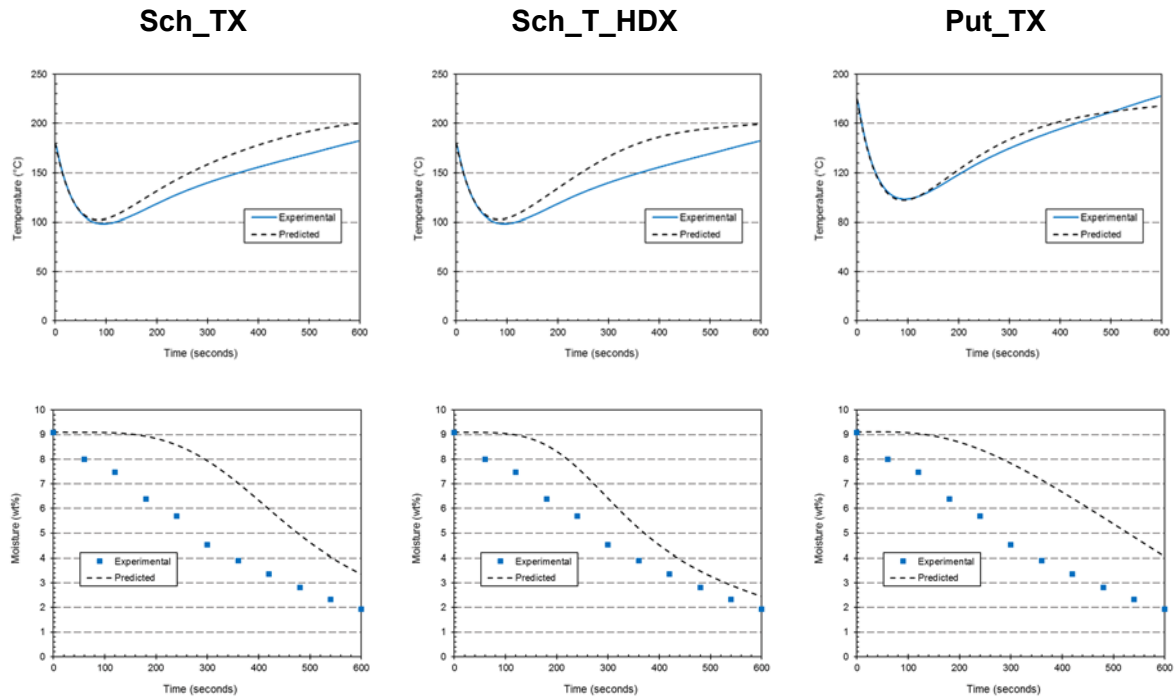


Figure H.2: Modelling validation results of all three models for a start of roast at 180 °C.

H.2.2 190 °C

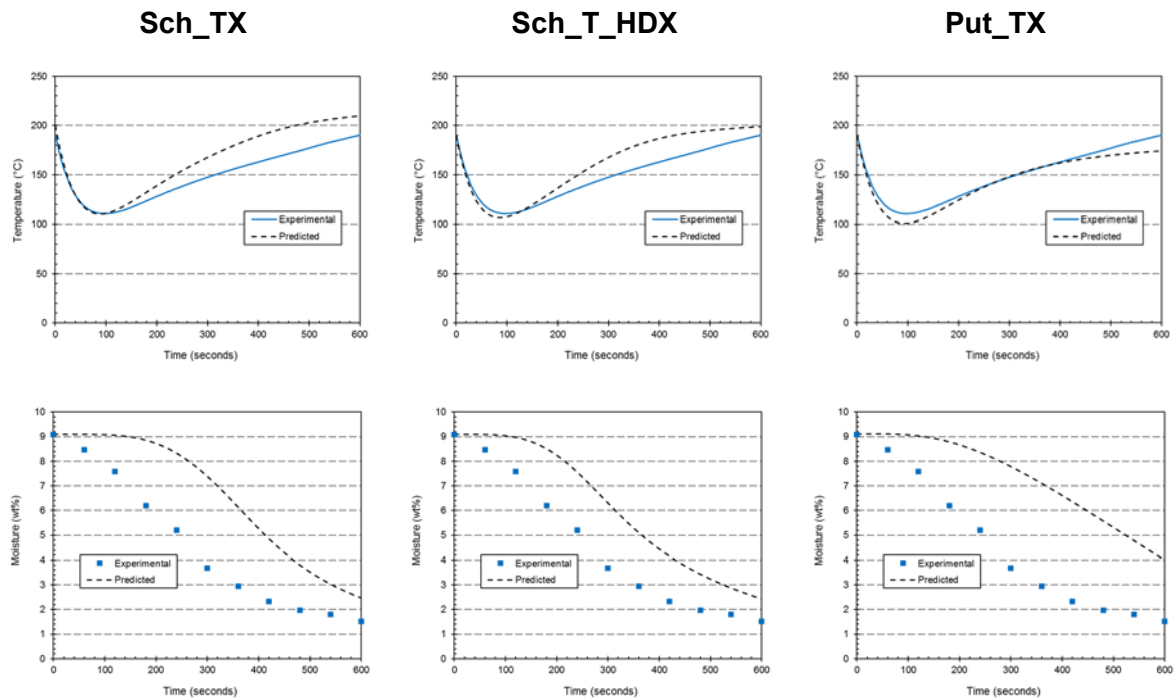


Figure H.3: Modelling validation results of all three models for a start of roast at 190 °C.

H.2.3 200 °C

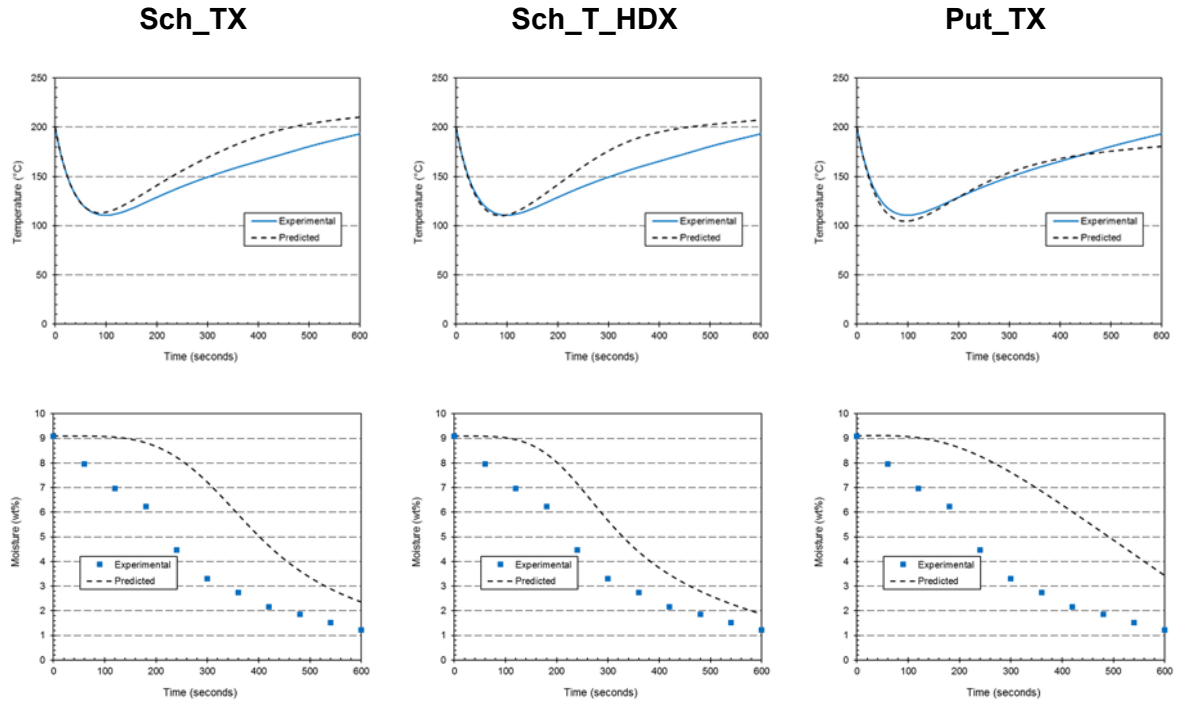


Figure H.4: Modelling validation results of all three models for a start of roast at 200 °C.

H.2.4 210 °C

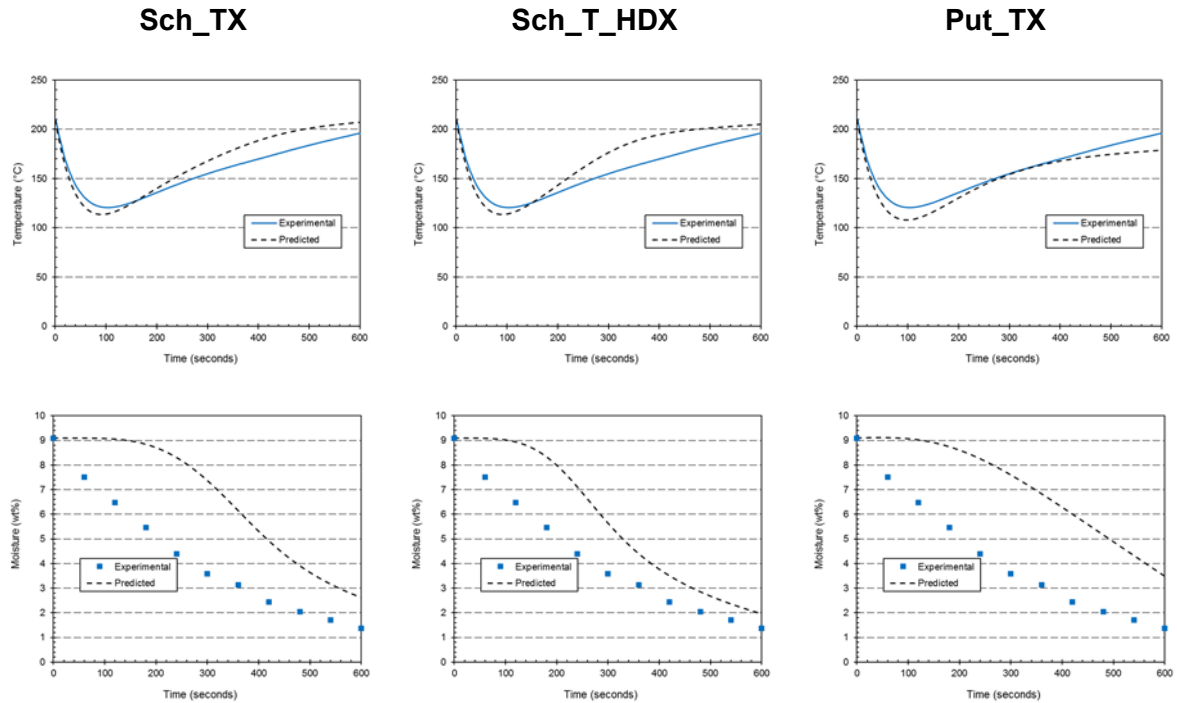


Figure H.5: Modelling validation results of all three models for a start of roast at 210 °C.

H.2.5 220 °C

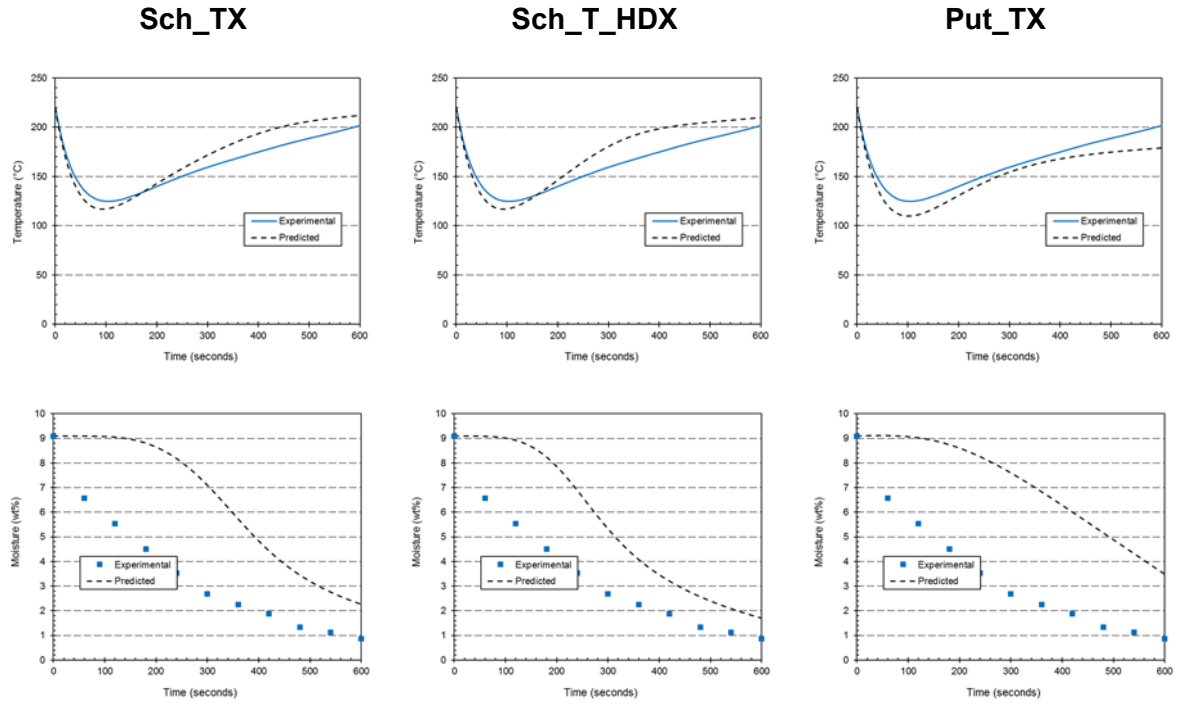


Figure H.6: Modelling validation results of all three models for a start of roast at 220 °C.

H.2.6 230 °C

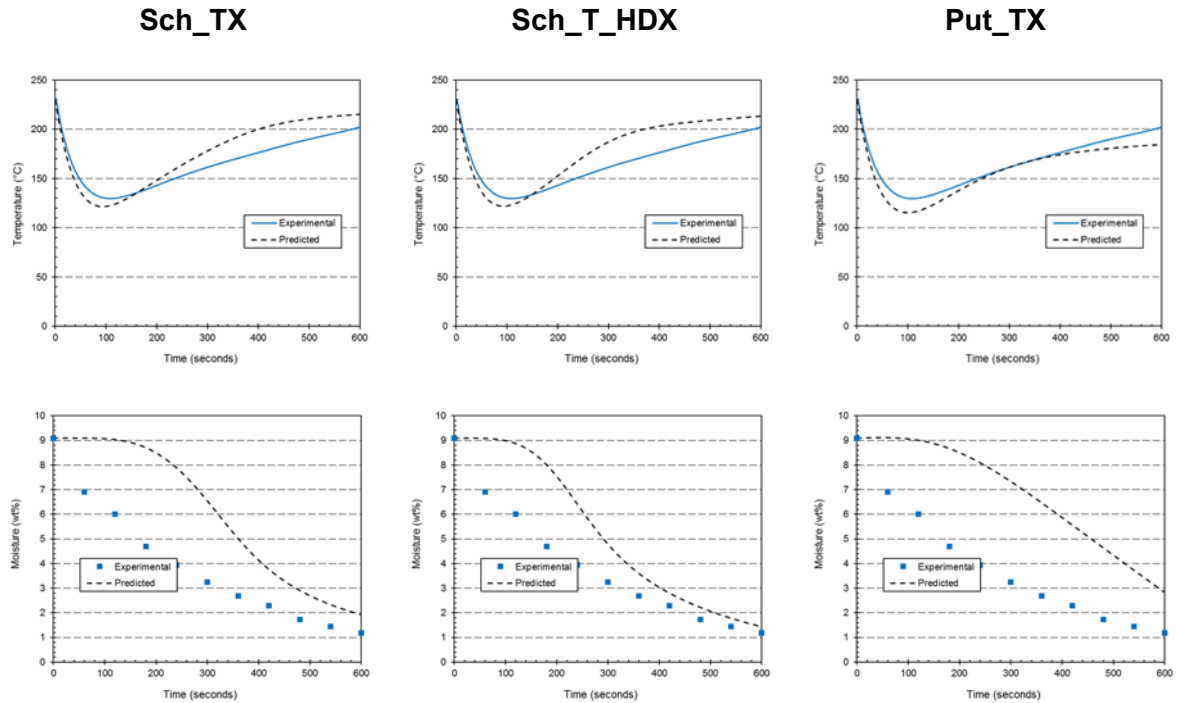


Figure H.7: Modelling validation results of all three models for a start of roast at 230 °C.

H.2.7 240 °C

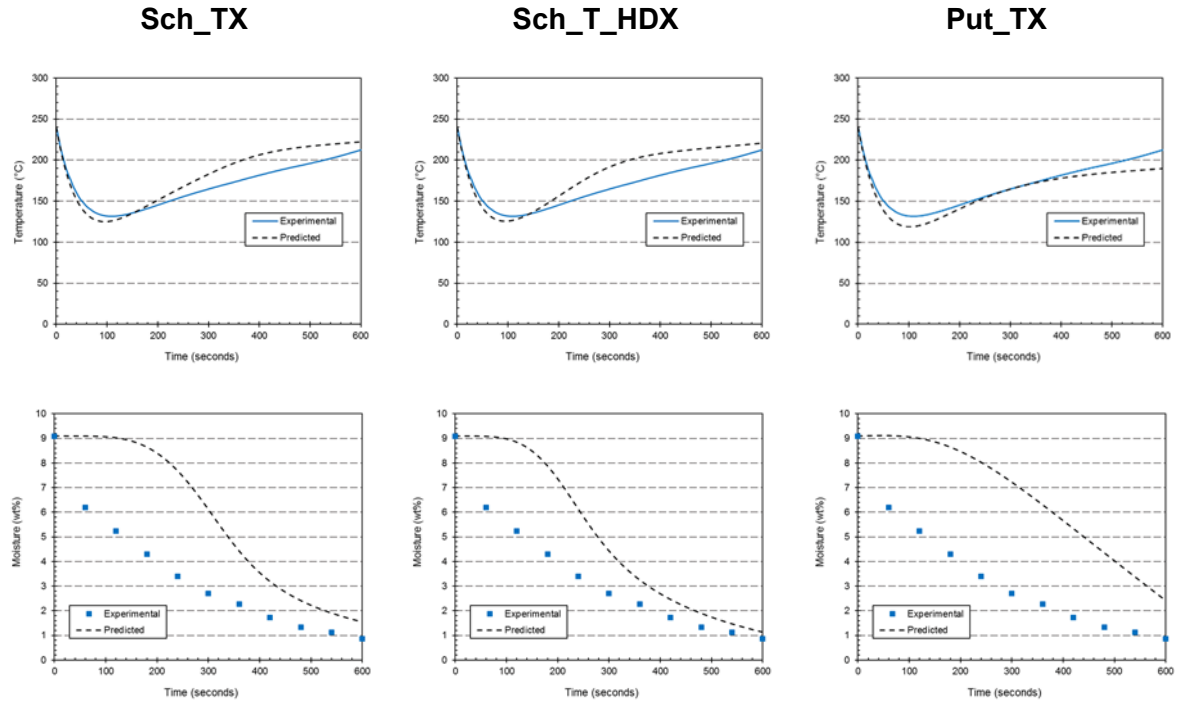


Figure H.8: Modelling validation results of all three models for a start of roast at 240 °C.

H.3 Validation results for roasting until second crack

H.3.1 180 °C

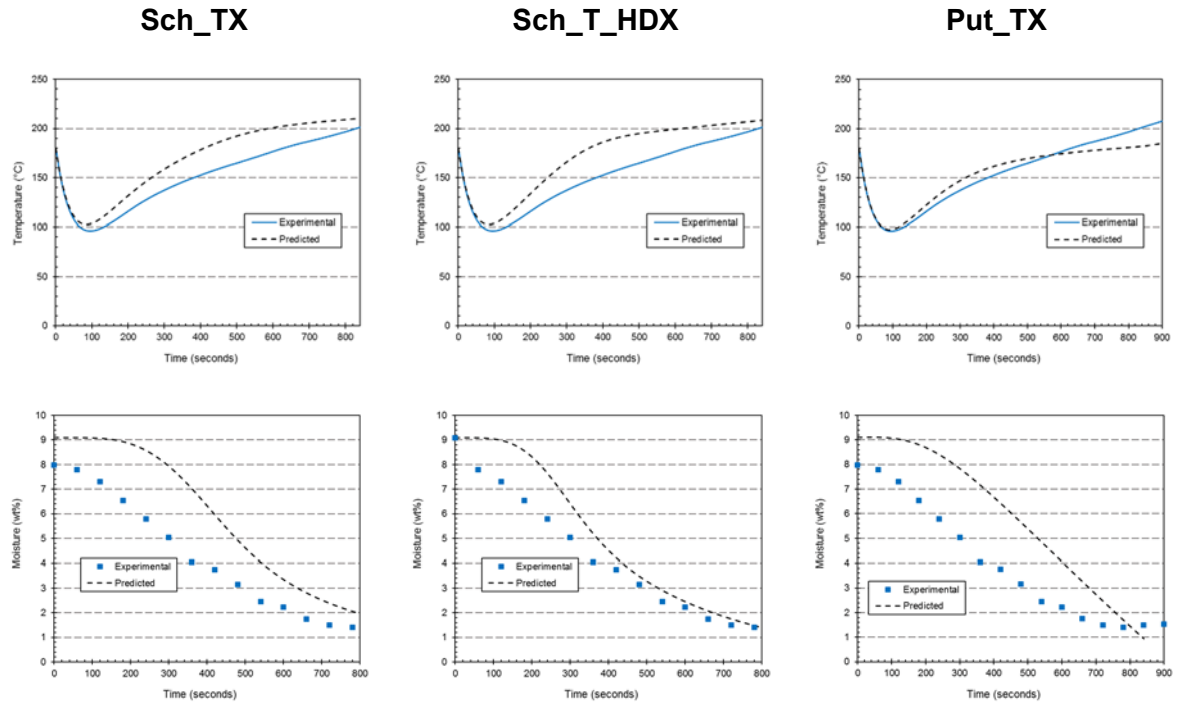


Figure H.9: Modelling validation results of all three models for a start of roast at 180 °C.

H.3.2 190 °C

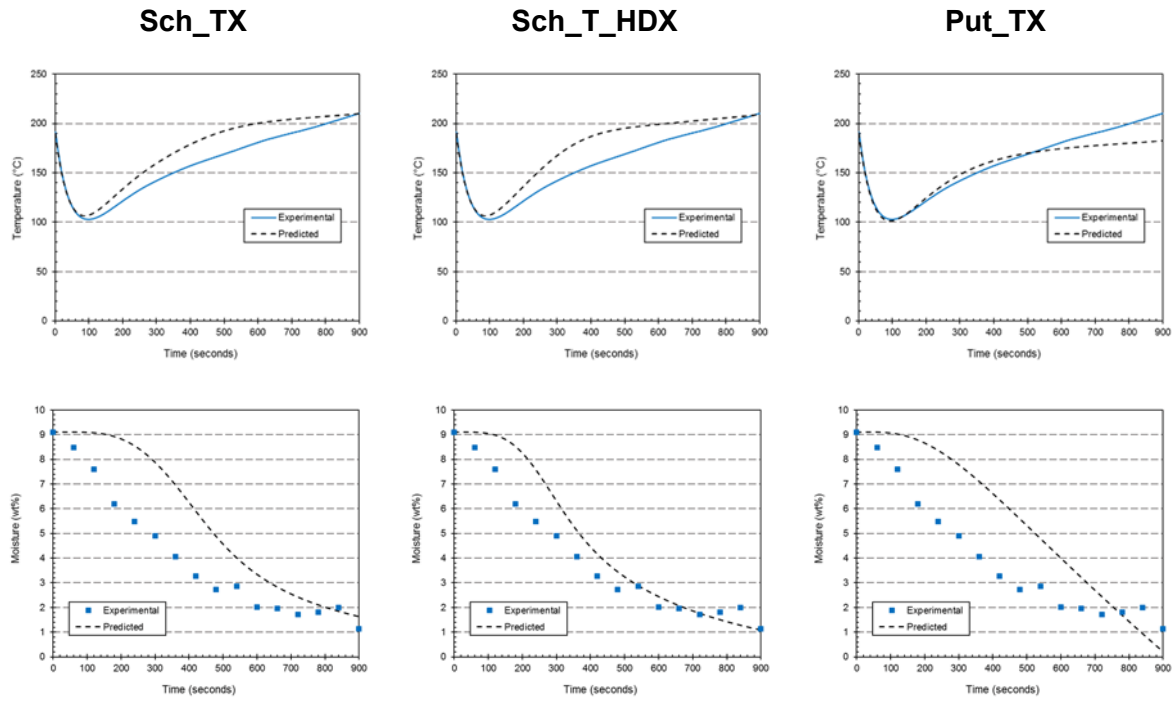


Figure H.10: Modelling validation results of all three models for a start of roast at 190 °C.

H.3.3 200 °C

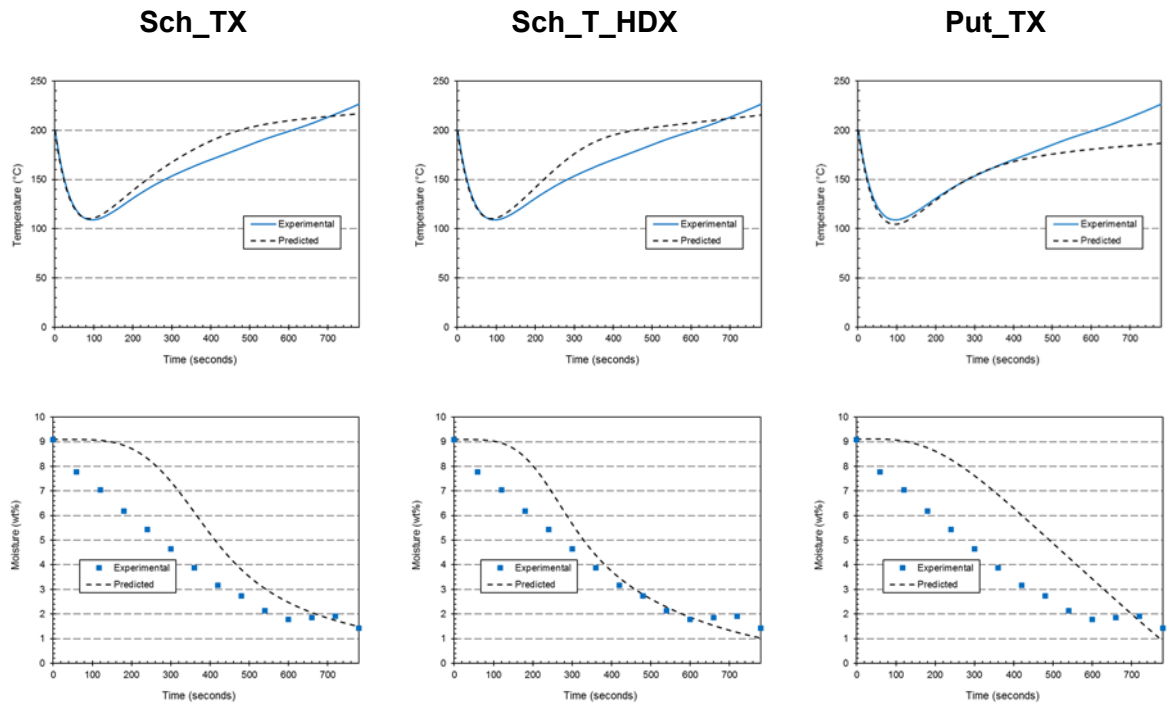


Figure H.11: Modelling validation results of all three models for a start of roast at 200 °C.

H.3.4 210 °C

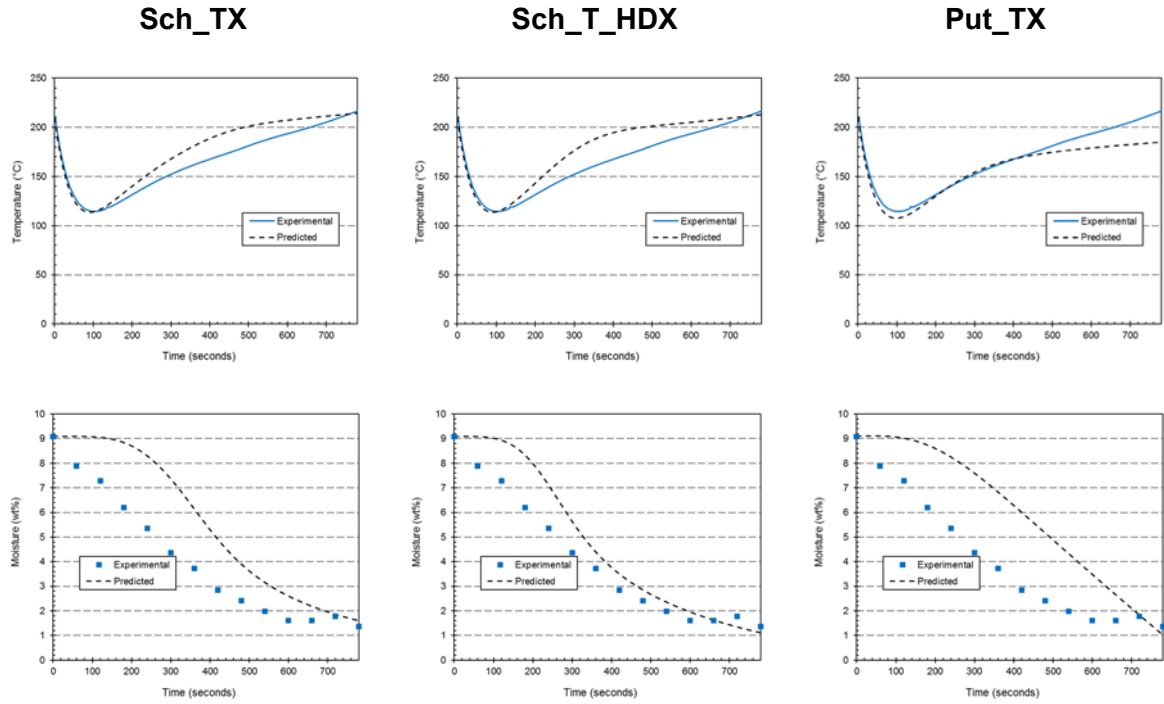


Figure H.12: Modelling validation results of all three models for a start of roast at 210 °C.

H.3.5 220 °C

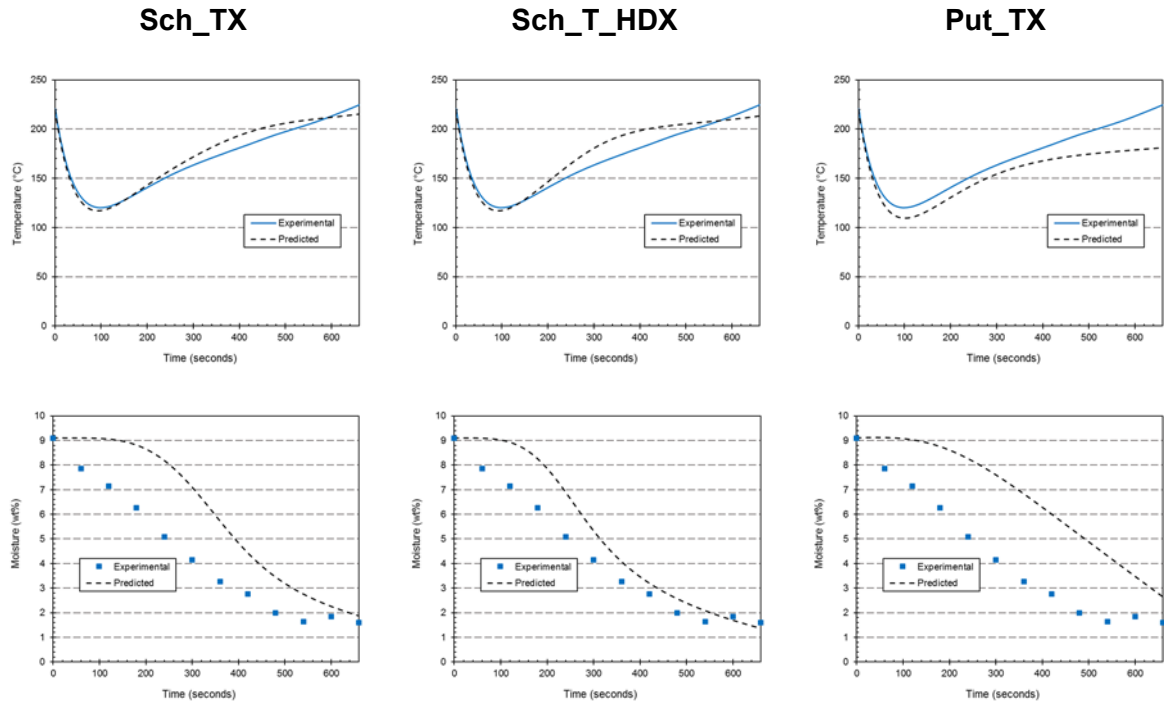


Figure H.13: Modelling validation results of all three models for a start of roast at 220 °C.

H.3.6 230 °C

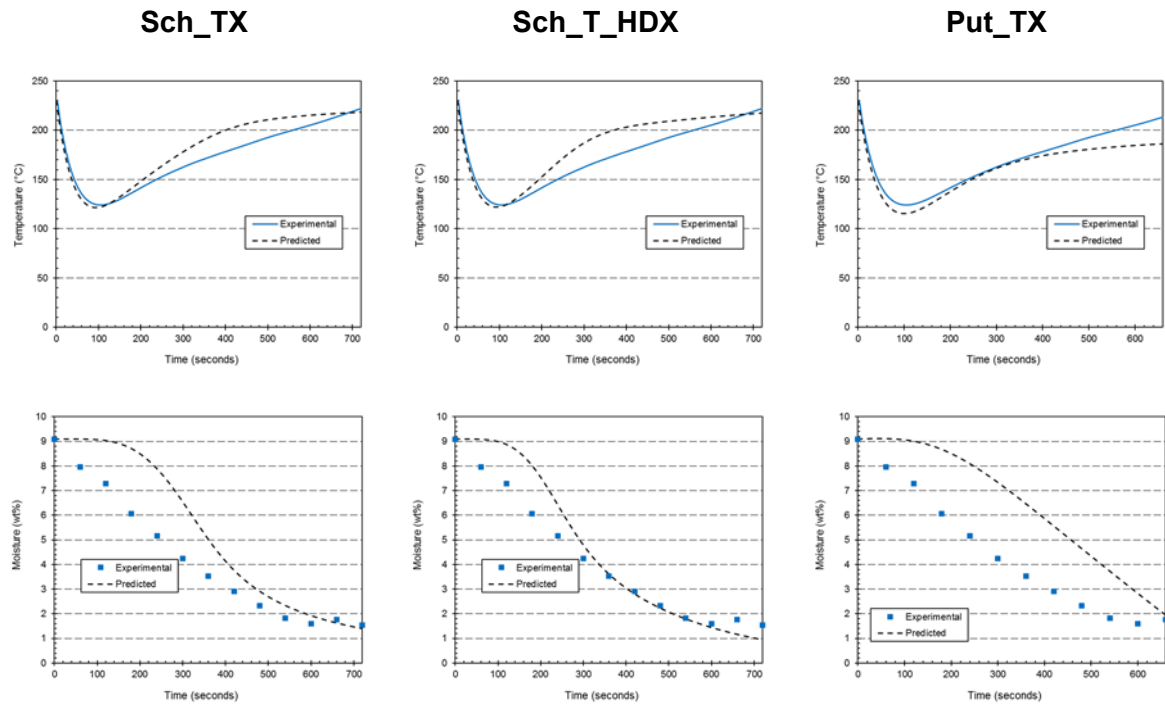


Figure H.14: Modelling validation results of all three models for a start of roast at 230 °C.

H.3.7 240 °C

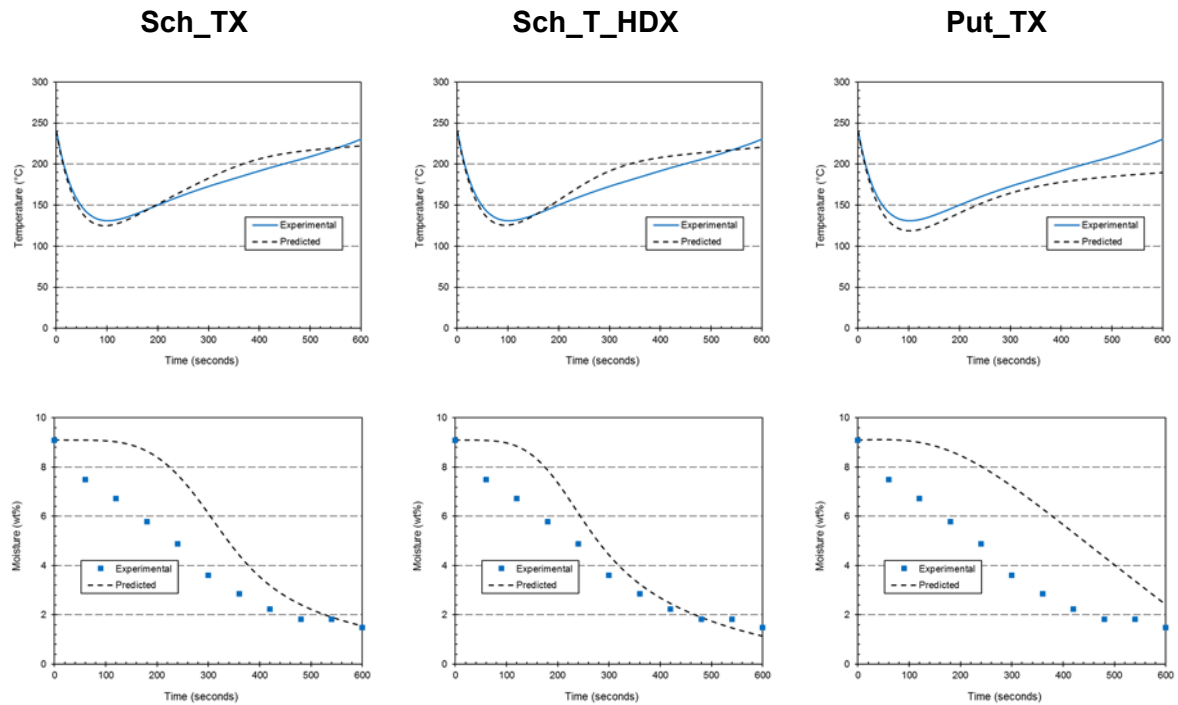


Figure H.15: Modelling validation results of all three models for a start of roast at 240 °C.

H.4 Validation results for roasting with 12.7 wt% green beans

H.4.1 190 °C

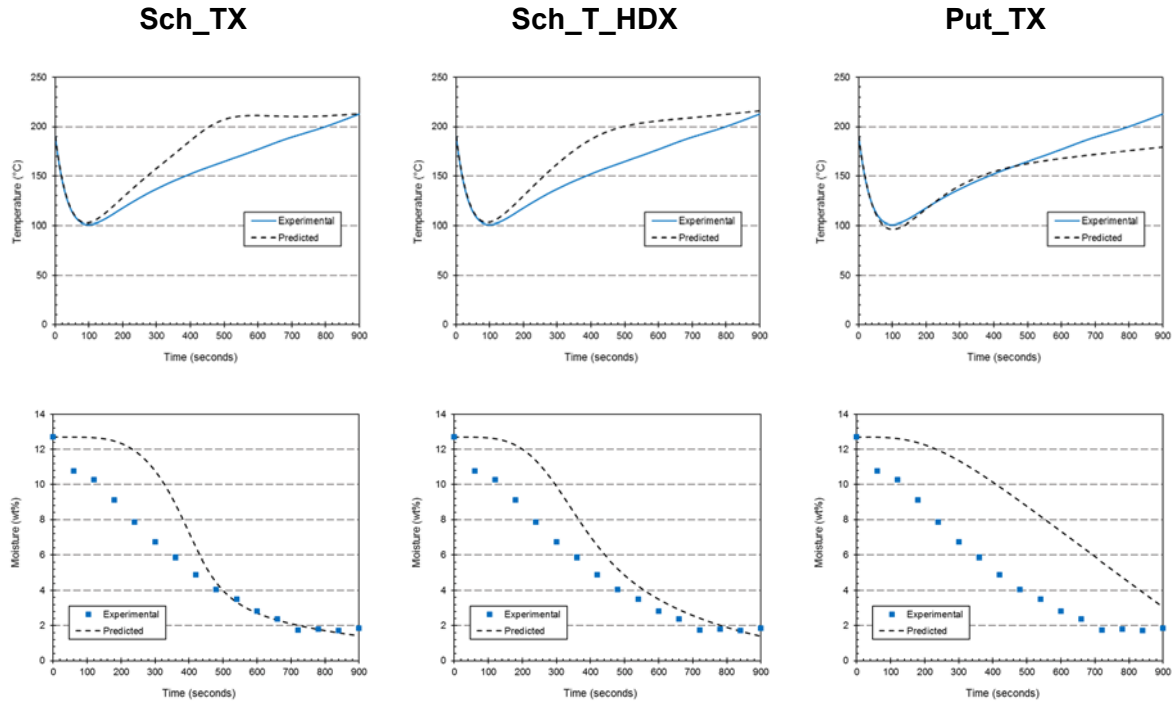


Figure H.16: Modelling validation results of all three models for a start of roast at 190 °C.

H.4.2 210 °C

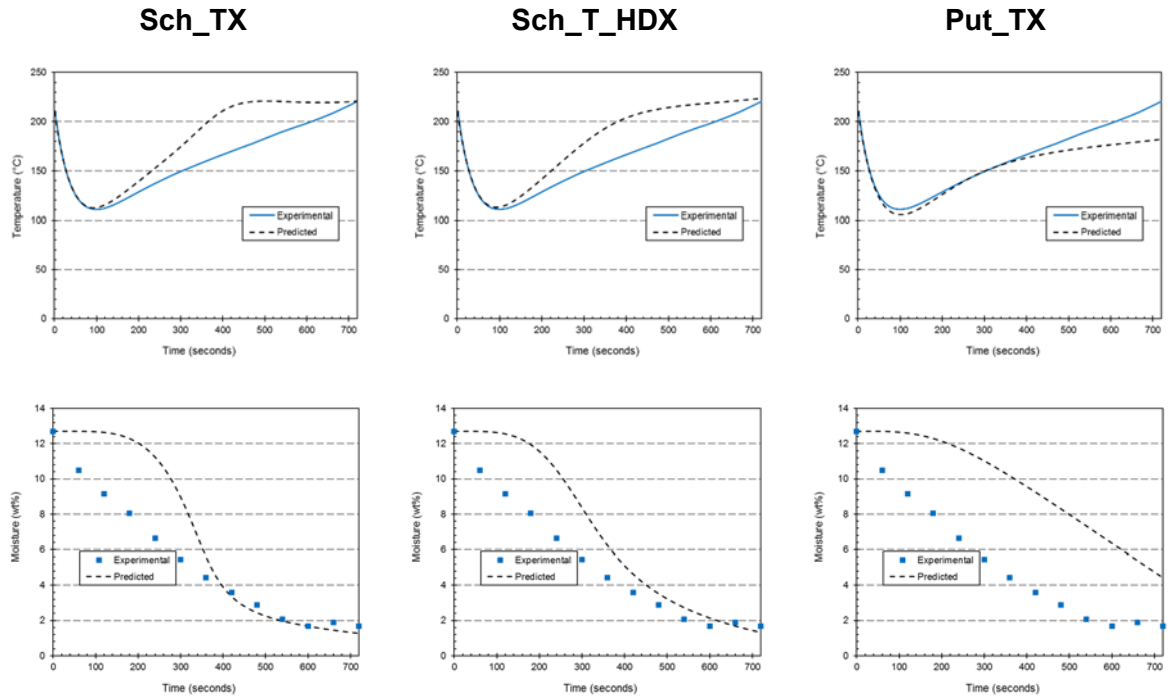


Figure H.17: Modelling validation results of all three models for a start of roast at 210 °C.

H.4.3 230 °C

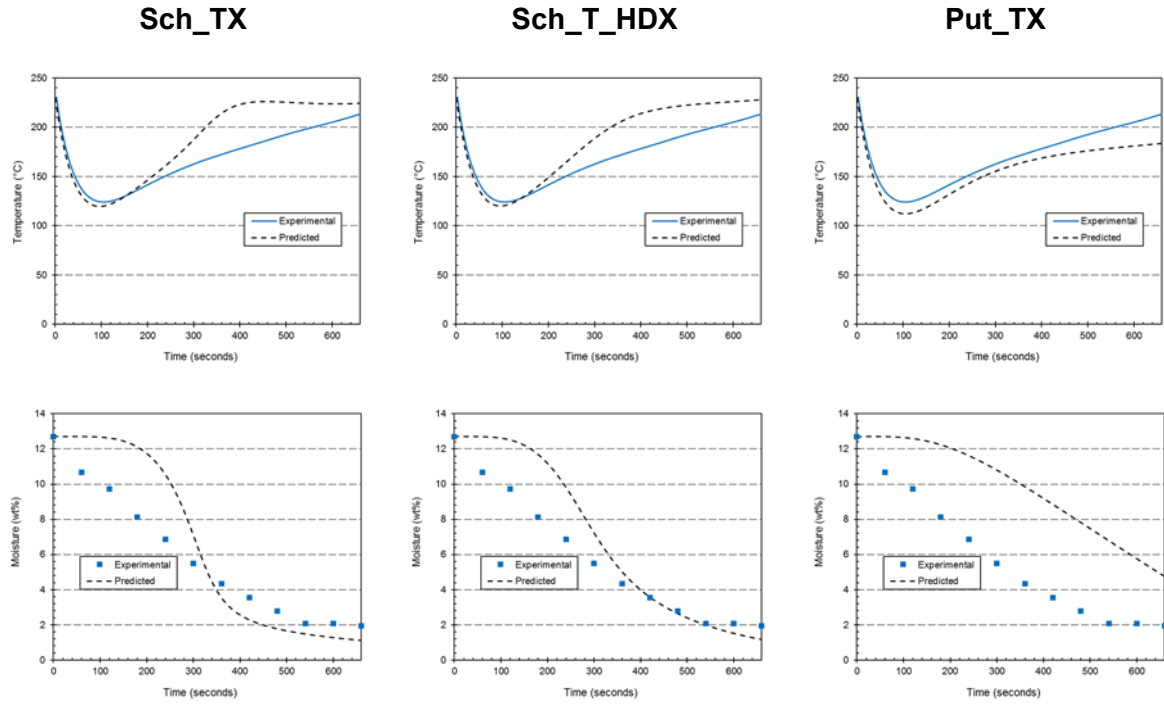


Figure H.18: Modelling validation results of all three models for a start of roast at 230 °C.

H.5 Validation results for roasting with 13.3 wt% green beans

H.5.1 170 °C

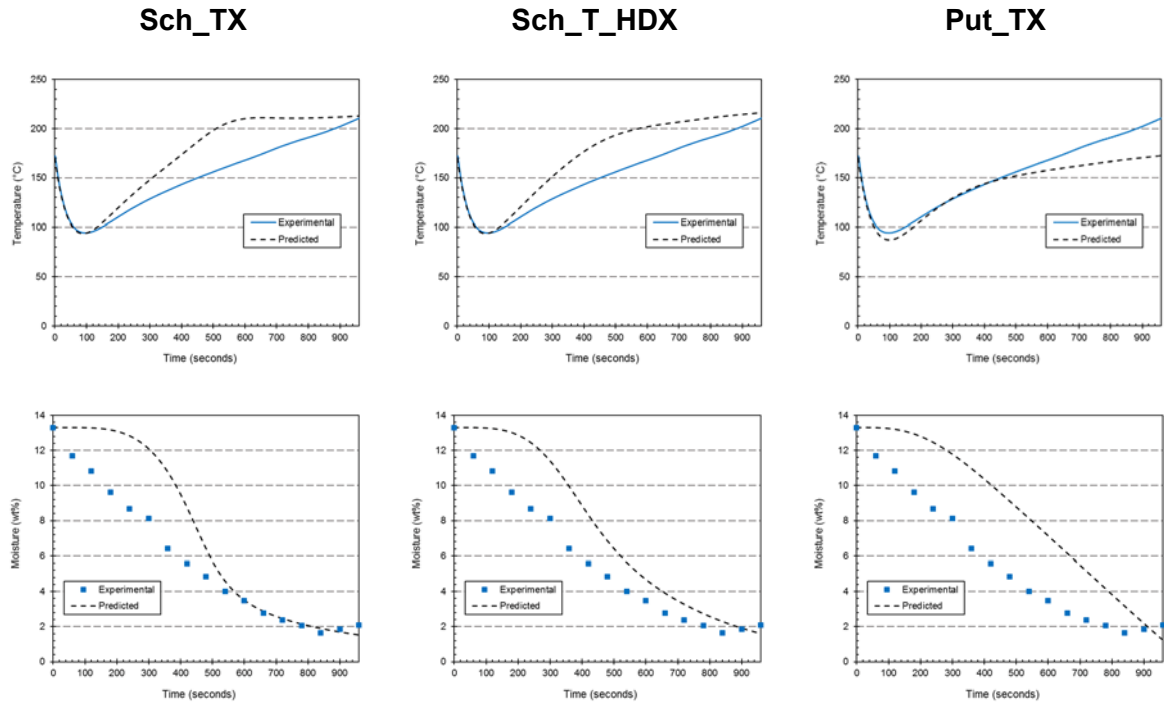


Figure H.19: Modelling validation results of all three models for a start of roast at 170 °C.

H.5.2 190 °C

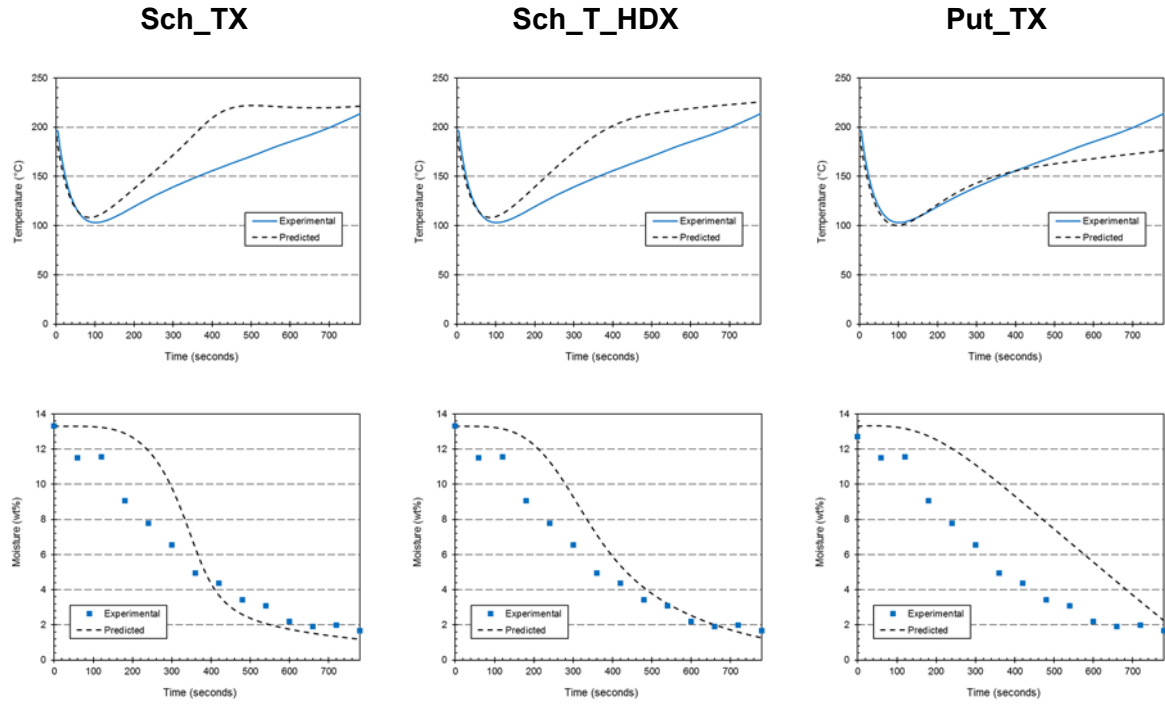


Figure H.20: Modelling validation results of all three models for a start of roast at 190 °C.

H.5.3 210 °C

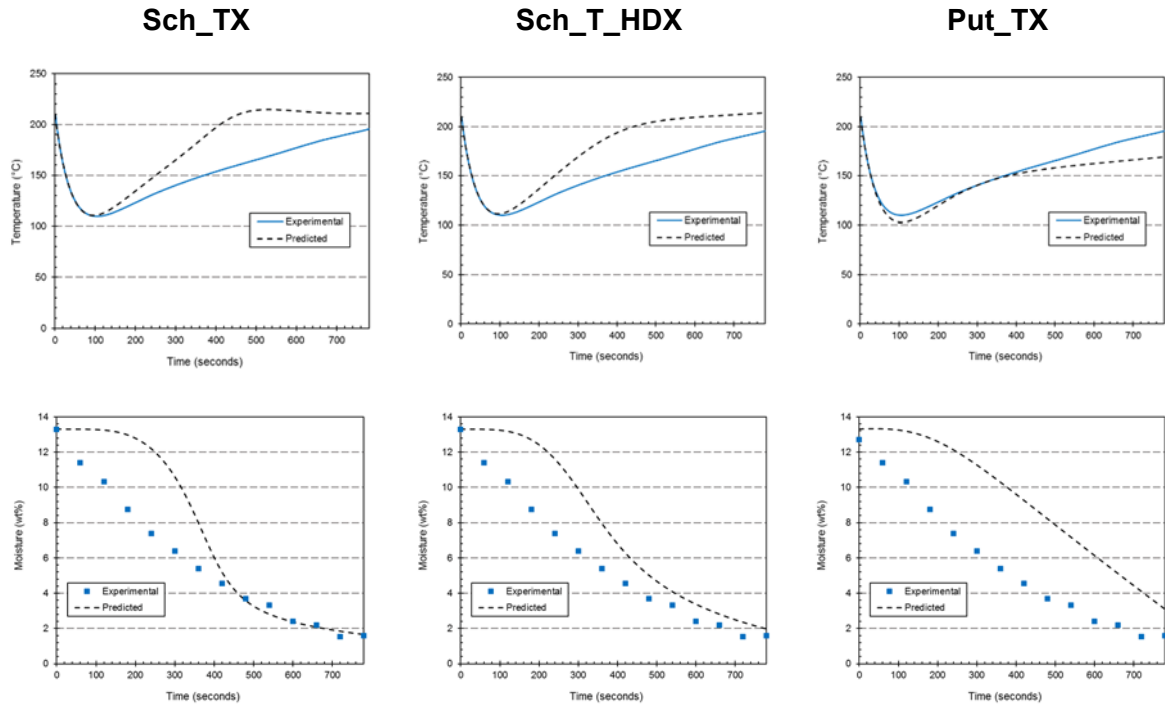


Figure H.21: Modelling validation results of all three models for a start of roast at 210 °C.

H.5.4 230 °C

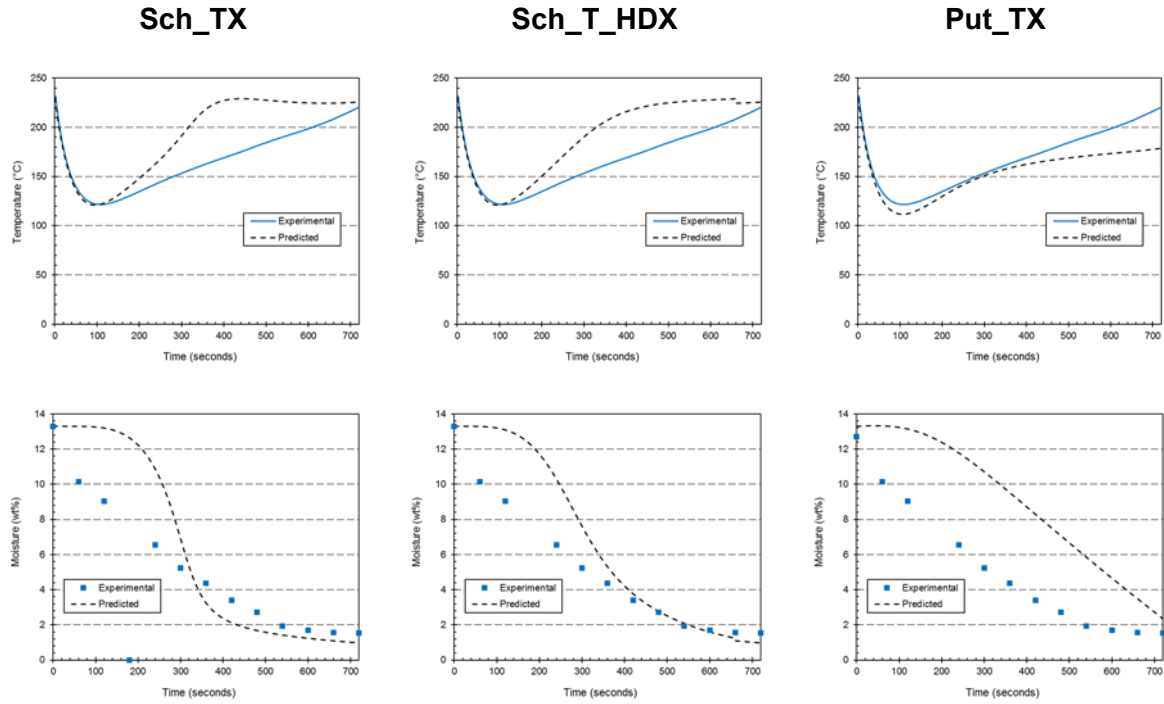


Figure H.22: Modelling validation results of all three models for a start of roast at 230 °C.

H.6 Validation results for roasting with 14.5 wt% green beans

H.6.1 170 °C

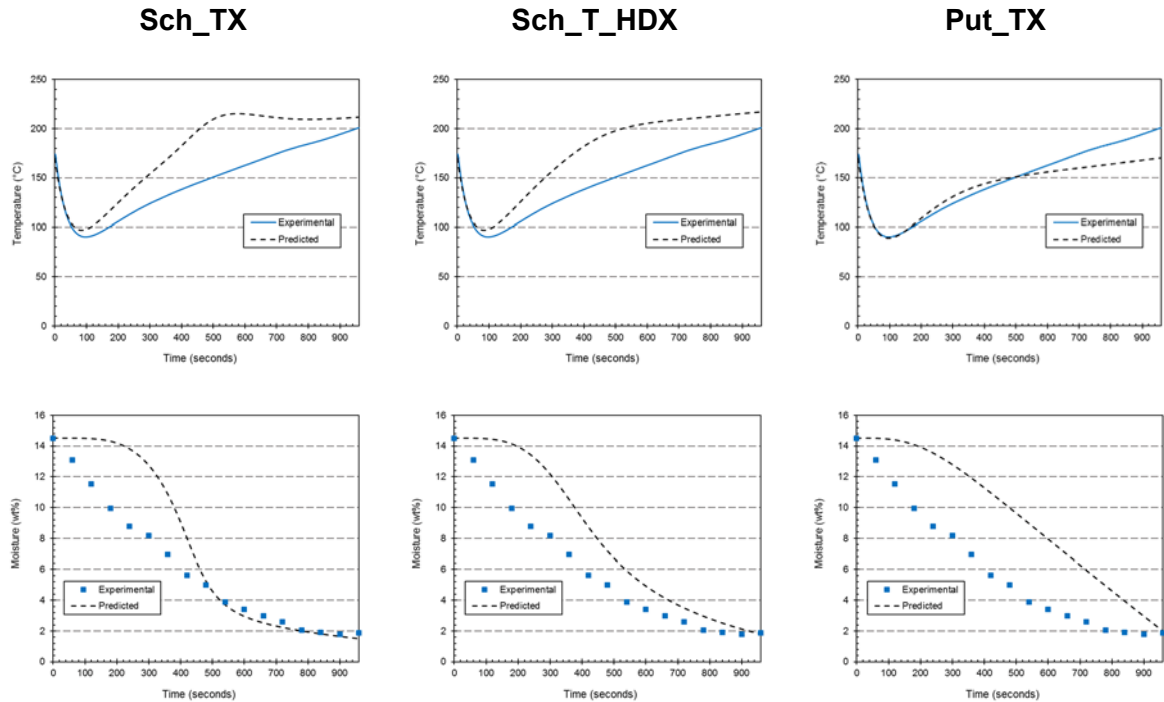


Figure H.23: Modelling validation results of all three models for a start of roast at 170 °C.

H.6.2 190 °C

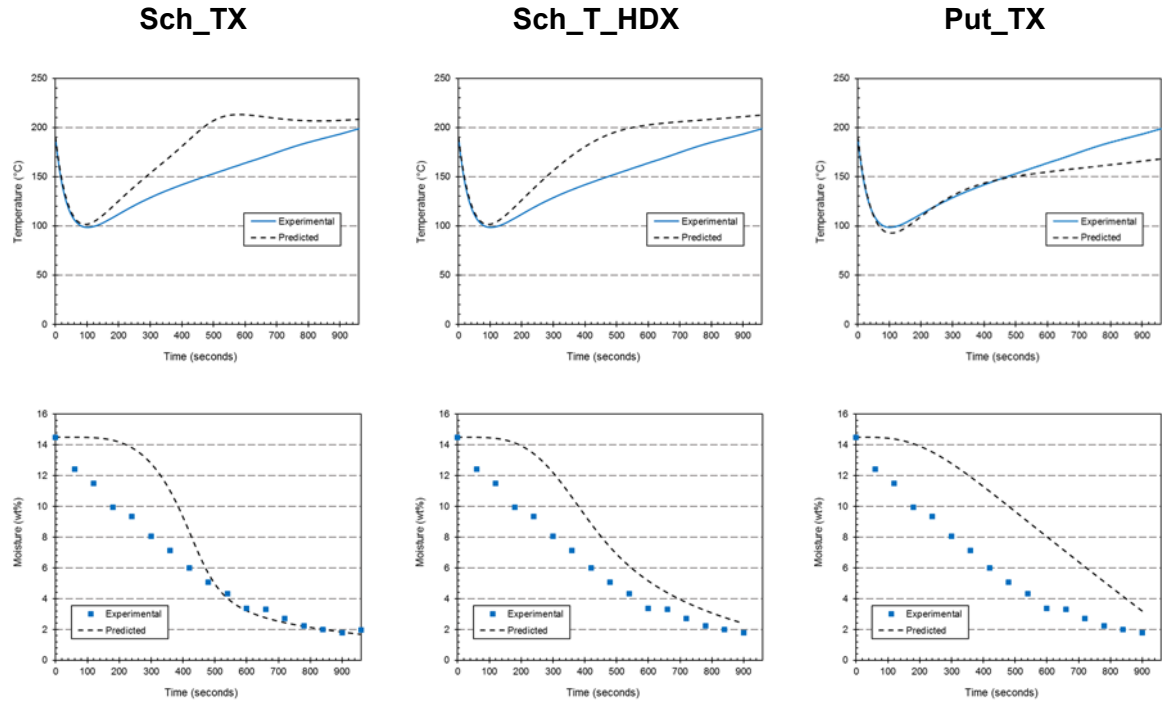


Figure H.24: Modelling validation results of all three models for a start of roast at 190 °C.

H.6.3 210 °C

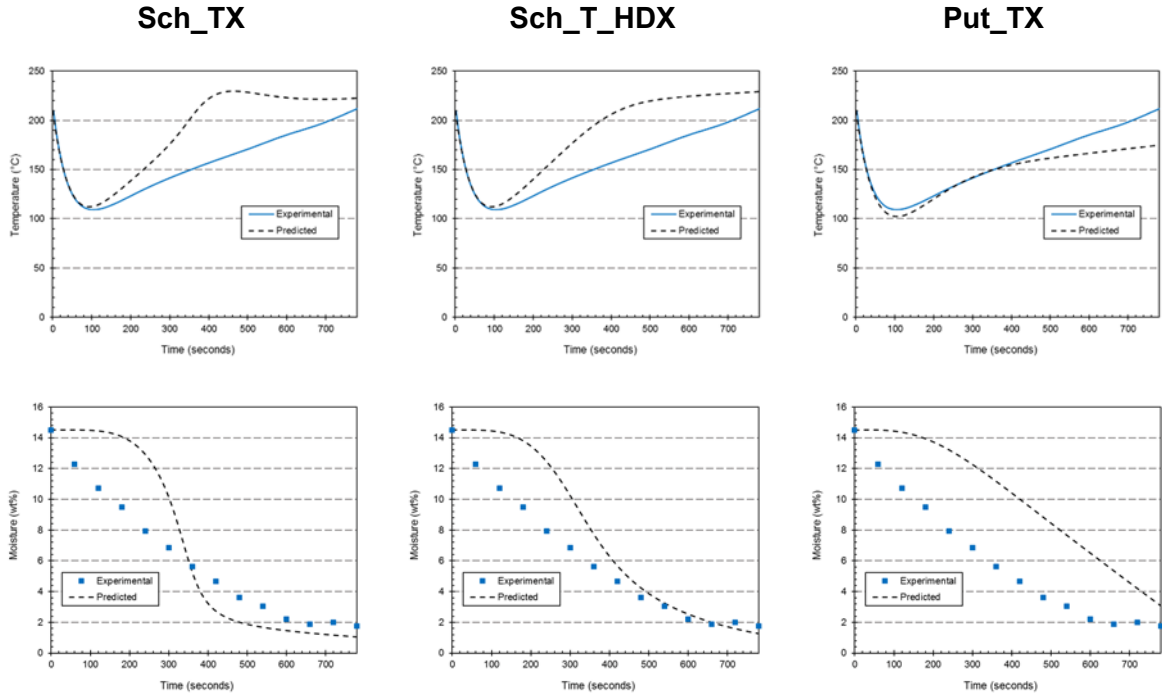


Figure H.25: Modelling validation results of all three models for a start of roast at 210 °C.

H.6.4 230 °C

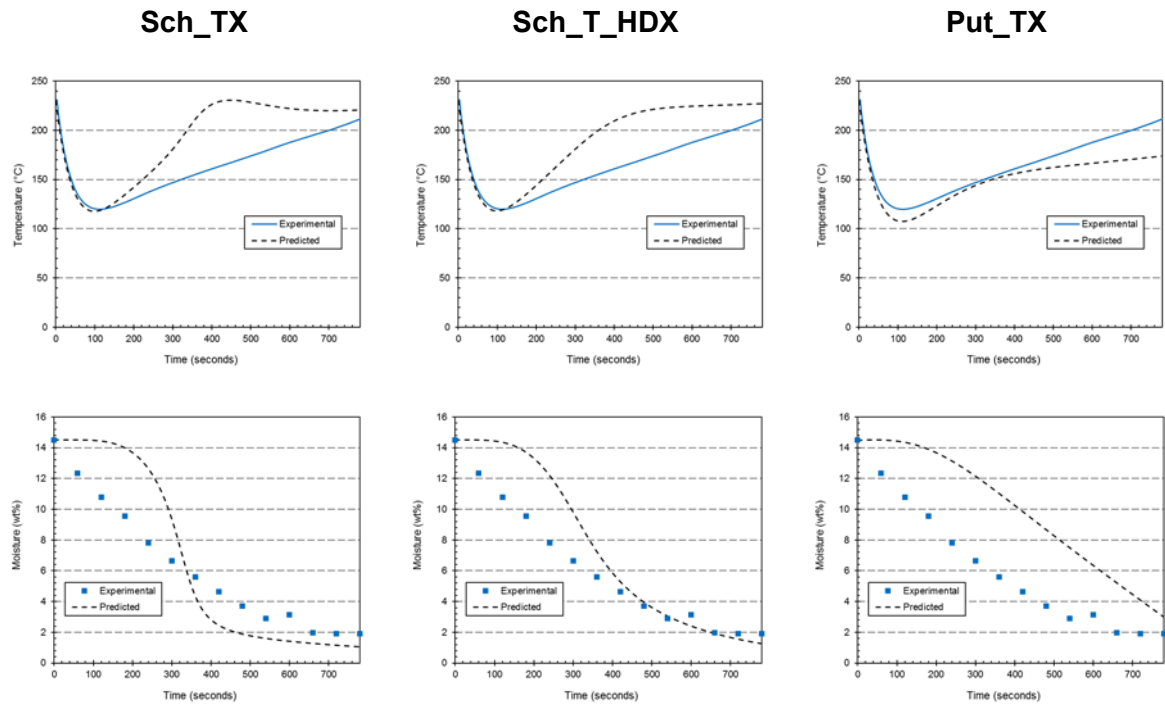


Figure H.26: Modelling validation results of all three models for a start of roast at 230 °C.