The Art of Coffee Roasting

Investigations into Sensor Development for the Application of Controlling Coffee Roasting

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Abstract

In this thesis, I investigate novel methods of sensing change in roasting coffee. Coffee roasting is a vital step in coffee's supply chain. It is the process that takes green coffee and transforms it via a series of many chemical and physical reactions to produce the flavours for which coffee is recognised. As of today, correctly roasted coffee has been an art. My work applies different methods of sensing to track various changes in coffee as it roasts with the end goal of automating the art.

The goal was to find an event or measurable phenomenon that could be used to detect when the roasting coffee has reached an ideal point, beyond which the beans would start to taste burnt. My investigations looked at various sensing methods. I expanded on three different areas of test: bean temperature, online moisture measurement using microwave resonance, and surface chemistry using Raman spectrometry. Using these different methods, I was able to produce novel and interesting measurements.

Each of the measurement methods performed satisfactorily and produced novel results. These results however did not produce the desired measurable event or independent characteristics. This meant that they were not able to individually solve the problem. However, their uniqueness and application flexibility would allow them to be used as elements in future roasting sensor systems.

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1 Thesis Summary

This thesis covers the inception, application, and evaluation of different sensor methods for measuring various changes in coffee while it is batch roasted. The goal is to autonomously create perfectly roasted coffee. The methods tested produced smooth near featureless progressions. These progressions were indistinguishable from other readily observable phenomena. Additionally, the measurements did not produce any repeatable transients that could be used to predict second crack.

Coffee roasting is the step in the coffee supply chain that creates the flavour that coffee is known for. It is therefore, a very important and valuable step in the process. It is not, however, straightforward to produce excellent quality roasted coffee. Roasting coffee well is often considered an art.

During roasting, coffee undergoes over two hundred different chemical reactions. By roasting completion, the coffee has lost around 15% of its mass, increased in size, and changed colour. The goal of an expert coffee roaster is to stop the process at a point that optimises desired flavours. Achieving an ideal roast is a goal that is further complicated because not all green coffee is created equal.

Coffee of varying origins behave differently and can produce different flavours during roasting. A coffee's origin is based on where the coffee was grown and how it was processed up to the point of roasting. Each coffee origin requires the roaster to do a test roast, to find out how best to roast that particular origin.

The goal of this work was to create a method which controlled the end of a roast to ensure an "ideal roast". During roasting, coffee passes some audible milestones, first and second crack. First crack is where the coffee pops in a manner like that of popcorn; the bean undergoes rapid expansion because of a build-up of various volatiles trapped inside the bean structure. Second crack comes after the main roasting reactions have been completed; at this point the reactions become so violent that they fracture the cell wall and can cause chunks of bean to break off.

For this work "ideal roast" is defined as the point just before second crack occurs and not after. Coffee roast past second crack starts to be considered burnt.

Additionally, coffee roasted past second crack starts to lose characteristic flavours unique to the individual coffee's origin.

The benefit of being able to do this detection would be a universal measure of roast completion. This would allow the roasting of good tasting coffee without professional expertise. This in turn would enable small, in home sized, automatic coffee roasters that would provide the final consumer a fresher coffee.

Considering the prevalence of coffee and coffee roasting, the scientific literature is thin. There are works that are focused on measuring roast progression in different ways including temperature, colour, surface texture, exhaust gas composition, or combinations of these. A solution to the problem this thesis sought to solve, a universal method of predicting second crack, was not found in the literature. Therefore, the focuses of this work are approaches that are previously unexplored in literature, that are then applied in an online batch roasting setting.

The methods chosen to look at were: a variation of bean temperature, microwave moisture measurement, and examining surface chemistry using Raman Spectrometry. In the temperature measurements, the coffee was roasted with a ramp temperature profile (different from what is seen in literature) which permitted the observation of the changing thermal reactions in the coffee. Using a microwave resonant cavity, allowed for the observation of the changing relative permittivity of the coffee during roasting; this in turn represented the coffee's moisture loss. Lastly, a method of observing the coffee's surface chemistry using Raman spectrometry was applied and evaluated.

1.1 Scope

The goal of this thesis was to "investigate automating the process of roasting coffee". After applying tight control to the roasting process by means of a fluidised bed, the outstanding problem became determining the roast end point. The task was then to implement and evaluate different measurement techniques, dealing with the engineering challenges involved with taking those measurements. Preferably the various techniques being tested would produce some new information on the roasting process as well as independent factors affecting the roast progression.

Each measurement method considered had to satisfy certain criteria. First, a measurement had to be physically possible in an online roasting environment. Secondly, the measurement needed to produce a meaningful result above noise. Thirdly, the measurement ideally would show something new. Additionally, particular consideration was given to the search for some previously unobserved in-roast transient (or "smoking gun") that could be used as a universal bench mark to track degree of roast.

The goal of this thesis was not to complete an exhaustive study of the behaviour of coffee beans under roast. The goal was to test novel methods of examining coffee beans under roast. A good example of a study looking at the physical and chemical changes produced in coffee beans during roast would be S.Schenker's thesis "Investigations into hot air roasting of coffee." [1].

1.2 Chapter Breakdown

Chapter Two provides a history of coffee and coffee processing. It sets the scene by providing a history of coffee. Then examines the process of getting coffee from farm to consumer. It looks at the value of coffee throughout the production process. Finally, it discusses the shift to small-scale coffee roasting and examines the importance and benefit of having coffee roasting closer to the consumer.

Chapter Three looks at the science and lore of coffee roasting. Due to coffee's wide consumption there is a large body of non-quality-assured information beyond what is found in scientific literature. The chapter looks at the published works related to coffee roasting and outlines important points from the wider body of coffee knowledge. It includes an outline of different coffee roasting techniques. The chapter concludes with an overview of various sensor approaches and discusses their respective viability.

Chapter Four looks at the construction of a fluid bed coffee roaster and thermal analysis of batch roasted coffee. A rudimentary method of calorimetry was preformed (during roast) which produced a measure of the coffee's load on the system. This characteristic was given the variable named "Bean Load". To better understand the bean load, a simple one-dimensional model was constructed.

Chapter Five looks at the use of a microwave resonant chamber to measure the changing moisture in coffee during batch roasting. These measurements were made by designing a special roasting chamber that acted as a single port microwave resonator. The roast chamber worked well for roasting coffee but did not make the ideal set-up for microwave moisture measurement. Therefore, a way had to be found to make this measurement in an environment aversive to microwave measurement.

Chapter Six looks at the attempt to measure the changing surface chemistry of the coffee beans using a Raman spectrometer. It starts with taking Raman spectroscopy measurements of single beans roasted to varying degrees in a static and controlled environment. It then describes modifications to the coffee roaster which allowed the use of an external probe from the Raman spectrometer. This setup allowed for measurements on coffee during fluidised operation. Measurements were done initially on pre-roasted coffee and then on coffee during roasting.

Chapter Seven concludes the thesis by summarising the conclusions drawn from the experimental work. The chapter makes suggestions as to how the methods could be improved with future work, primarily by being tested in combination with each other. The chapter and thesis conclude with some final thoughts and recommendations.

1.3 Thesis Contribution

This thesis has made the following contributions:

1.3.1 Coffee Thermal Analysis

1. Roasting coffee in a fluid-bed allowed for a ramp temperature profile which is uncommon in the literature.
2. The ramp temperature profile allowed for a calculation of a variable "Bean Load". The bean load variable showed the changing relative endothermic and exothermic activity in the coffee beans during a coffee roast.
3. Using bean load, 'first crack' was observable.
4. Using bean load, 'second crack' was not observable or predictable.

1.3.2 Microwave Aquametry

5. A fluid bed roasting chamber allowing online microwave measurement was designed.
    a. The microwave measurements were made in a system [coffee roasting chamber] that was not ideal for microwave aquametry. The limitations on this system included:
        i. Changing sample temperature.
        ii. Sample moving in an uncontrolled manner.
        iii. Changing sample size.
6. The limitations in making a microwave measurement using this roasting chamber required a measurement and data processing approach not seen in the literature. This approach was to:
    a. Find a resonant peak that moves in a consistent pattern when a sample in the chamber is perturbed.
    b. Test how various variables (such as moisture content and temperature) affect the chosen resonant peak.
    c. Stack sequential peak measurements in a matrix producing a data set that can be viewed as an image.
    d. Use image processing techniques to isolate the moving peak.
    e. Draw conclusions based on earlier tests.
7. The data collected from roasting coffee using this method showed the effect of changing permittivity in the coffee as it roasted. Initially permittivity increased as the coffee temperature increased, but then decreased as the temperature stabilised and moisture loss started.
8. Using this microwave aquametry technique, 'second crack' was not predictable.

1.3.3 Raman Spectrometry

9. Measurements were taken using a Raman spectrometer in a stable environment on series of coffee beans roasted to increasing degrees.
10. These measurements did not show any Raman spectra; they did show a progressively increasing level of overall fluorescence.
11. A coffee roasting fluid bed setup was constructed to allow the Raman spectrometer to make online measurement of coffee while it roasted. This

required addressing the problem of making spectroscopy measurement on large moving particles.

12. This setup was shown to be able to reproduce results aligning with measurements taken in the stable environment.
13. Online measurements showed an increase in fluorescence —like the static test— as the roast progressed.
14. Using this technique 'second crack' was not predictable.

1.3.4 Published Works

The following papers have been produced from this work with a further paper being prepared for submission.

- Kelly, C.B.D., Scott J.B. (2014) Online Thermal Analysis of Batch Roasted Coffee Beans: Conference proceedings ENZCon 2014
- Kelly, C.B.D., Scott J.B. (2015) Does Anyone Need a Coffee? Online Microwave Moisture Measurement of Roasting Beans: Conference proceedings APMC 2015
- Kelly, C.B.D., Scott J.B. (2015) The Coffee Roaster's Paradox: Conference proceedings ENZCON 2017

2 The Coffee Problem

2.1 Origin of Coffee by Historical Reference

Coffee needs very little introduction — it is enjoyed by millions of people every day, making it one of the world's most consumed beverages — but the origins of coffee are often underappreciated. Legend has it that coffee was first discovered by Ethiopian shepherds who noticed their animals acting more energetically after eating the berries from the coffee bush. The discovery soon spread to the local monastery. The monks realised that consuming the seeds gave them more energy and focus in late night meditation and prayer.[2] This origin tale may just be legend but it is known that coffee was first cultivated on the Arabian Peninsula and started to spread in the Middle Ages, first to India and then to the rest of the world.[3] It is believed that the seeds were consumed as food before the beverage became popular.

The original brewing practices would have been similar to what is known as Turkish coffee today. Turkish coffee — rather than referencing the coffee's geographical location — is a method of preparing the coffee drink. It involves grinding roasted coffee into a very fine power, adding water, and then bringing the water to boiling or nearly boiling.[4] This method produces a strong coffee with the ground coffee left in the bottom of the cup.

Since its first discovery, coffee has spread to all corners of the earth. The process chain followed in preparing and then consuming coffee has modernised and changed, however the basic principles remain the same.

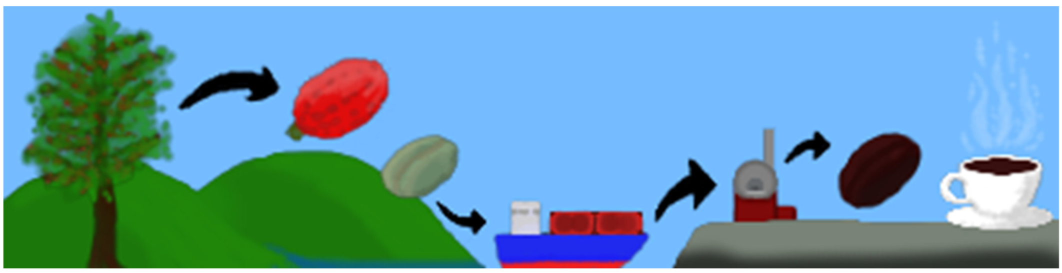


Figure 1. The coffee process and origin of coffee

2.2 Coffee Process Chain

Modern coffee processing moves coffee from plantations in the tropical highlands to consumers' cups. There are five links in this process to bring coffee from farm to cup. These links are:

1. Growing the coffee
2. Processing the green coffee
3. Transporting the coffee
4. Roasting the coffee
5. Grinding, Brewing, and Infusing the coffee

There are numerous different sources covering the production and consumption of coffee. Clarke et al.'s book from 1987 "*Coffee Volume 2: Technology*" [5] is one of the earliest and most well referenced works looking into the science and technology involved in processing coffee. Another very good resource on the processing of coffee is Illy's "*Espresso Coffee*" [6]. Finally, Buffo et al.'s paper "C*offee flavour: an overview*" [7] contains a good look into the science and chemistry of roasting coffee. The following section draws a lot of reference from these works.

2.2.1 Growing Coffee: Geography and Biology

In modern times coffee is mostly grown in tropical highlands — in a region sometimes called the coffee belt.[8] The coffee belt is the region between the tropics where all of the world's major producers are located (Figure 2). For example, Brazil — the world's largest producer of green coffee — is located in the coffee belt.

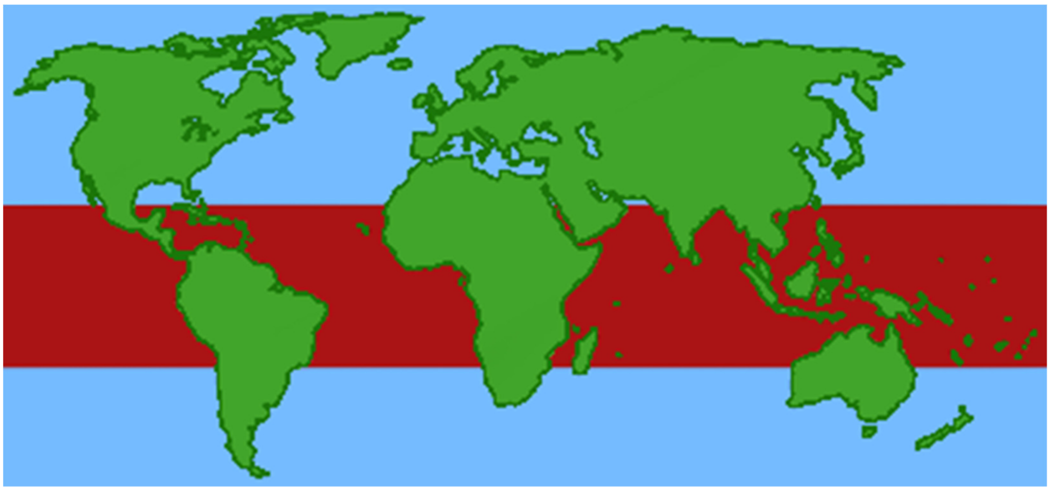


Figure 2. The coffee belt. [9] The region between the tropics where most of the world's coffee is grown.

Coffee is grown as a shrub or small tree; these trees produce clusters of red cherries (Figure 3). Each cherry contains two small seeds commonly referred to as coffee beans.

Figure 3. Cluster of ripe coffee cherries on the tree

2.2.2 Cherry Processing, Bean Drying, Parchment Hulling, and Grading

The seeds are extracted from the cherry using one of two main commercial methods: wet processing and dry processing. Dry processing involves drying the coffee cherries and then milling them to remove the husk of the cherry leaving the bean. Wet processing consists of soaking the cherry in water and then forcing the cherry through a screen producing a bean that still has pulp on it. The pulped bean is soaked again and the pulp ferments loosening its hold on the bean. The pulp can then be washed off the bean leaving the bean clean for drying. Although the wet processing method is more complex it produces more uniform coffee than dry processed coffee.[5]–[7], [10]

2.2.3 Transport

Most coffee is grown in countries other than where it is consumed. All coffee will, therefore, experience long distance transport and shipping. Typically, green coffee beans are shipped in jute sacks inside shipping containers. The coffee is expected to spend an extended period in transport, therefore the method of containment can affect the quality and taste of the final coffee. For example; a local professional coffee roaster mentioned anecdotally that coffee of the same variety and of the same region transported in different bags changes the final flavours of the coffee. To this end there are various steps and standards that are observed when transporting coffee. [11]

Figure 4. Sacks of coffee beans ready for transport [12]

2.2.4 Roasting Coffee

Coffee roasting is the other step in the process that is vital to getting a cup of coffee and it is the central idea covered in this thesis. It is the roasting process that takes the green coffee seeds (commonly referred to as “beans”) and produces all the characteristic flavours for which coffee is known. Roasting occurs while exposing the beans to temperatures of around 200 – 250 Celsius.[5]–[7], [13]–[17] It takes a person experienced in coffee roasting to be able to produce and reproduce well-roasted coffee.[6]

Figure 5. Pan roasted coffee [18]

2.2.5 Grinding and Brewing/Infusing

Coffee is ground to increase the surface area that is in contact with the brewing water. The grind size is carefully selected because of its effect on the final brew strength. A fine grind is used to produce a stronger cup. Grind size is also chosen depending on the brewing method used. Brewing method and grind size selection is related to the time water is in contact with the coffee. For example, in espresso coffee — shown in Figure 6— the water is forced through the coffee; this means that the water is only in contact with the coffee for a short period of time, thus a finer grind is used. [6]

Once coffee reaches our shores — a long way from where it is grown — the seeds are roasted, ground, and brewed. The brewing and preparation of coffee has come a long way from its original Arabic style. Modern brewing practices are designed to remove the grind from the final brew while still producing a good flavour. Some examples of modern coffee brewing include:

- Espresso: a method of forcing a near boiling water through a cake of ground and compressed roasted coffee.
- Plunger or French Press: ground coffee is mixed with hot water and when the brew is completed a filtered press is passed through the brew separating the grinds from the brew.
- Filter method: hot water is passed through ground coffee sitting on filter paper.

Now processed, the coffee's value has been increased by several orders of magnitude and it can finally be consumed.

Figure 6. Various brewing methods. Turkish, vacuum flask, French press, espresso machine. [19]–[22]

2.3 Economics of Coffee

Each step in the process increases the value of the coffee. Roasting represents a significant price increase. Roasting can double the value by weight of the coffee (Figure 7). The requirement of a skilled roaster is one of the biggest contributors to this value increase.

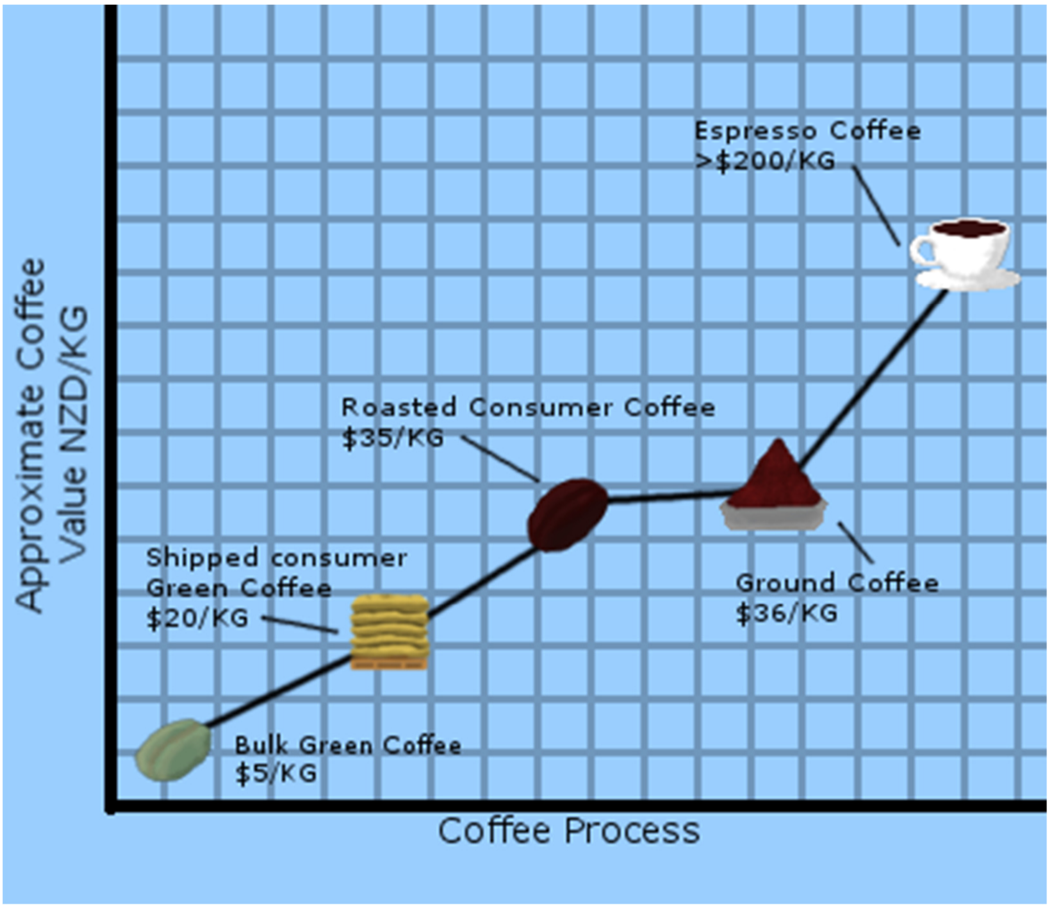


Figure 7. Illustration of the coffee roasting process and it effect on coffee value

From the graph (Figure 7), mild Arabica coffee can be purchased bulk on the commodities market for around US $4.50 per kg (US $0.03 a cup). For the average consumer wanting to purchase and roast their own green coffee the price triples to approximately US $14 per kg (US $0.09 a cup). Each step in the chain adds value and, therefore, extra cost to the coffee. Economically, it makes sense to process coffee in bulk and sell the fully processed product to the consumer. Unfortunately, bulk production does not see the best quality coffee reach the consumer.

2.4 Bringing Coffee Home

2.4.1 Coffee Origin and its Effect on Roasting

When is a coffee roast finished? An expert coffee roaster's goal is to produce well roasted coffee. They do this by controlling the roast temperature and observing the coffee, waiting for the ideal place to end the coffee roast. An expert is needed to roast coffee because coffees with different origins behave differently when roasted. The origin of a particular coffee is everything that has happened to it on its journey from coffee plant to the point where is it is roasted. Often quoted as the biggest factor affecting a coffee roast is the coffee's geographic origin. The geographic origin does affect the roast but it is not the only factor to have a noticeable effect. Factors that affect the origin include the weather of the particular growing season, the method used to extract the bean from the cherry, how well the coffee is sorted, and even the type of sack in which the coffee is transported.[11] With all the factors that can affect a coffee's origin (and therefore roast behaviour) and with a lot of coffee being produced with third world production standards it can be difficult to obtain coffee that behaves consistently when roasted. This means that every batch of coffee needs to be test roasted by an expert before an ideal coffee can be produced.

2.4.2 The Problem with Coffee

On top of requiring an expert to roast it, coffee's other big problem is that it loses quality and flavour once roasted.[6] A rule of thumb is that roasted coffee should be consumed within three days of its being roasted for optimum quality. There are methods that can help extend this such as hermetically sealed bagging but all roasted coffee has a shelf life. The problem is worse when extended to ground coffee; ground coffee should be brewed within a few minutes of grinding in order to produce the best tasting coffee.[6] This means that the closer you can get these processes to the consumer the better quality their coffee will be.

2.4.3 A Small-Scale Shift

Coffee is still, for the most part, roasted in large batches by companies such as Nestlé [23], [24], but most cafes and coffee lovers will find a nearby coffee roaster to ensure a fresh roast. With modern consumers wanting higher quality coffee, the processing of coffee is moving closer and closer to the consumers' homes – as evidenced by the increasing number of tools for grinding and brewing roasted coffee readily available for home consumer application. For example, small coffee grinders are now common, so that the grinding can then happen just before brewing. Home espresso machines and combination grinder espresso machines are also readily available for home brewing, although they are still relatively expensive.[25], [26] Specialty small scale home coffee roasters are also available (Figure 8). They allow the coffee enthusiast to roast their own coffee very close to brewing. However, whereas grinding coffee is relatively easy, roasting coffee takes a lot more experience and effort. The tools to roast green coffee are straightforward: All that is required of the person roasting green coffee is a method of heating the coffee to a roasting temperature (about 250 C).

Figure 8. Comparison of commercial coffee roasting machine (left) with two home roasting machines (right).

The benefits of roasting coffee at home are twofold. First, a consumer can save as much as 80% on the cost of coffee (Figure 7). Secondly, the final flavour of the coffee is improved by roasting the coffee closer to consumption. Even with the tools being available, home coffee roasting has not taken off. The reason for this is also twofold. First, it adds an extra step in producing the coffee, making it less convenient. Secondly (and most importantly), it requires a level of expertise and practice to produce a coffee worth drinking. The average consumer does not have the time, money, or will to bother with learning a new skill to roast their own coffee. Solving the problem of requiring a skilled roaster would allow for the creation of a device that can bring coffee roasting to the home consumer.

3 The Science and Lore of Roasting Coffee

Coffee's extensive consumer base and audience produces a large amount of information. When approaching a topic as broad as coffee the fields of knowledge that should be considered are equally broad. For the purposes of this thesis the information has been loosely divided into scientific facts and community lore. The science (not surprisingly) is the information from the scientific community. This knowledge is focused around the "How" of coffee and coffee roasting. The "Lore" encapsulates the knowledge and experience from the wider coffee roasting community. Lore is more interested in making a good coffee than understanding the mechanics behind it. As the goal is to roast a good coffee, knowledge from both these fields is important. This chapter looks at pre-roasted coffee in more detail leading into an examination of a coffee roast from the perspectives of both these fields. It also covers some of the common roasting methods used in coffee roasting.

3.1 Pre-Roast Coffee/Coffee in General

3.1.1 The Plant

The coffee plant is a native to tropical areas in Africa with wild *Coffea canephora* being found in forests of Guinea and Uganda. The tree will freely grow to 4–6m for *Coffea arabica* and 8–12m for *Coffea canephora*. Depending on the harvesting method, however, the trees are kept around 2–3m tall for commercial production. [5], [6], [27]

3.1.2 The Cherry

The coffee bean that is used in the creation of the brew grows in pairs inside a red cherry from the coffee tree. The outer skin of the cherry is removed by either dry or wet processing.[5], [6], [10] Dry processing is the easier and cheaper of the two methods: it requires simply drying the coffee, under the sun or a manmade heat source, then removing the husk by mechanical agitation. In contrast, during wet processing most of the outer layer of the cherry is removed before drying.

Wet processing starts by receiving the cherries into a tank of water. This is used to remove floating cherries that are damaged or dried on the tree. After being received the cherries are pulped. The pulping process removes the exocarp (silver skin) and mesocarp (pulp). The next step is fermentation. This stage is designed to loosen the hold of mucilage from the bean. A subsequent washing stage then removes the mucilage. Finally, the wet processed beans are dried. Wet processing is done because the process produces a higher quality end product.

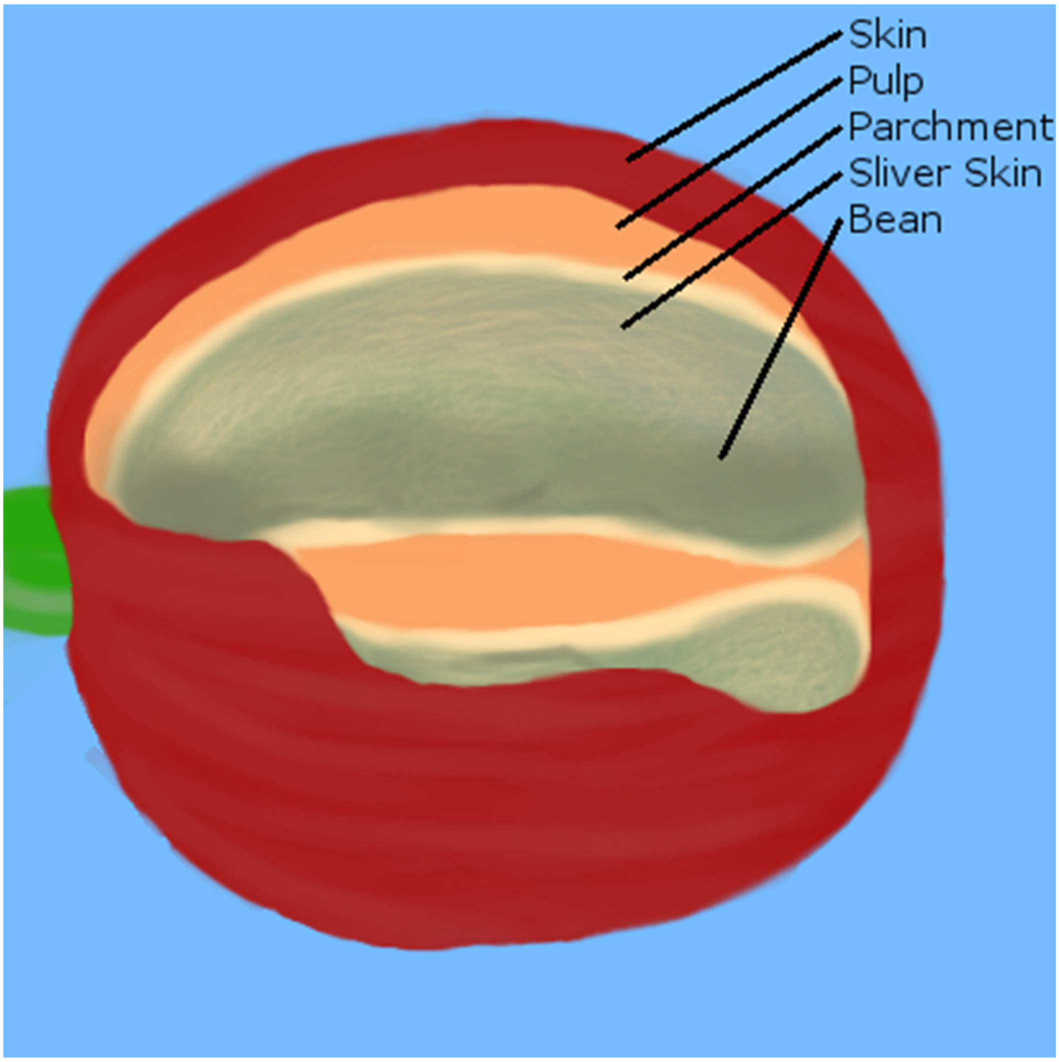


Figure 9. Diagram of a coffee cherry, (based off diagram in Coffee Volume 1: Chemistry[28])

3.1.3 The Coffee Bean

The coffee beans are typically sorted in a grader with hole sizes ranging from 10/64 of an inch (3.96 mm) to 19/64 of an inch (7.54 mm). The result at this point in the process is the green bean. The green bean contains the same amount of caffeine as roasted coffee. However, green coffee is not consumed because it lacks the characteristic coffee flavour that is introduced through roasting. The roasting process is affected by the different characteristics of the green bean. The geographic origin of the bean is one of the largest contributors to the characteristics of the green coffee. The reason for this difference in characteristics is believed to be the climate where the coffee is grown, e.g. increased rain fall can cause higher moisture content in the green bean.

3.2 The Science of Coffee Roasting

Coffee roasting, as described in the introduction, is the process of heating green coffee beans to high temperatures to produce the flavours usually associated with the coffee beverage. During the roasting process, a coffee bean undergoes many chemical and physical changes. These changes are often used by professional coffee roasters to indicate how far the coffee is through the roasting.

3.2.1 The Roast Progression

As coffee roasts, it progresses through three distinct stages in roast development. The stages are: the initial heating and dehydration phase, the roasting phase, and a burning or charring phase. The changes happening to the coffee show which stage the coffee is in.

The green coffee that starts a coffee roast is as the name suggests, a pale green colour. The green coffee beans are still wrapped in a husk (silver skin). The beans are around 4 – 8 mm long and contain around 10 – 15% water. [5], [6] Heat is applied to the green bean and the first roasting stage begins. [7]

The initial stage consists of the dehydration of the green coffee. The moisture levels in the coffee start to drop. The green colour starts turning yellow. The husk comes off — as chaff — leaving the yellowing grassy smelling bean. This initial stage ends with first crack. First crack is a violent release of built up water pressure like that seen in popcorn. The coffee's pop is not as dramatic as popcorn's but it does lead to an increase in the size of the bean. At the end of the first stage the coffee has grown, lost its husk, and started to turn brown.

The second stage starts after the first crack — this is known as the roast phase. At this point, most of the water has evaporated and the temperature of the coffee has reached a point where the roasting pyrolytic reactions begin. It is the reactions that happen during this phase that develop the flavours, scents, and colour for which coffee is known. During the roast phase over two hundred different reactions occur. Throughout the roast various volatiles are produced and expunged from the coffee beans. Early roasting is characterised by the Maillard reaction followed by caramelisation. As this reaction occurs, the colour of the bean changes from yellowy brown to the darker brown that is characteristically recognised as coffee. Coffee's strong colour change is commonly used as a measure of how well roasted the coffee is.[15], [29], [30] The colour has been used as a method to control the end of the roast.

The second phase — the roast phase — ends with second crack. Unlike first crack, second crack is caused by a pyrolytic reaction.[7] Second crack can cause chunks of the coffee bean to break off from the cracking. Second crack also causes the coffee bean's cell walls to rupture leading to the oils trapped in the coffee to seep out. As the roast continues into its final stage the charring and burning continues. The coffee beans go from dark brown to black.

Coffee roasting is ended by cooling the coffee. Ideally, this cooling is done rapidly so that the roast does not progress further than expected. Methods of cooling usually depend on the method of roasting. In a commercial drum roaster, the coffee is dumped from the roaster into a cooling tray. Other methods include spraying the coffee with water and pumping cold air through the coffee.[31]

3.2.2 The Not So Science of Coffee

Coffee roasting is a chemically complex process. [1], [5], [6], [13], [14], [32]–[34] The coffee bean undergoes numerous chemical and physical changes.[1], [5], [6], [14] The bean changes in size and colour, produces and loses different volatiles, and produces the well-known coffee flavour.[1], [30], [33], [34] The coffee roasting process is well known. The practice of roasting a good tasting coffee, however, is very subjective and often answered with less scientific vigour or quality assurance.

3.3 The Lore of Coffee Roasting

To the end consumer, coffee roasting is more about making a good tasting coffee than understanding the science and chemistry of roasting coffee. The understanding and knowledge of coffee roasting lore looks at coffee roasting through a different lens. This body of knowledge is focused on understanding the type and flavour of coffee that will come out after roasting. Looking at the coffee roasting process from the coffee drinker's perspective, the same science has a different meaning.

3.3.1 Degree of Roast, Roasting, and End Point

The goal of the master coffee roaster is to heat coffee beans in a manner that will develop specific desired flavours then bring the roast to an end before any unwanted flavours are developed. The end point is usually referred to as the "degree of roast".[35] The degree of roast can loosely be defined as the extent to which a coffee bean has been roasted. The problem is that the definition is not universal. If the degree of roast is defined by the colour of the bean (as is common in industrial practice [36]) then the roast is ended when the bean reaches a predefined colour. This method works if the same beans are roasted the same way. However, if the origin of the beans, the method of roasting, or the heating profile is changed, the colour will not correctly define the roast.[16] As of today there exists no solid or agreed upon definition of the degree of roast.[6], [7], [13] So how does a coffee drinker roast coffee? And what do they look for?

3.3.2 Roasting of a Drinkable Coffee

Again, it starts with pale green coffee beans. The questions to ask at this stage are: Where was the bean grown and what was its origin? Coffee can be ground and brewed at this early stage. The coffee will have the same stimulant effect as fully roasted coffee because of the caffeine; however, it has none of the flavour for which coffee is famous. Therefore, the initial heating and dehydration stage is not of much interest as it does not produce any of the desired flavours.

Once first crack has happened more interest is taken. Between the first and second crack is where all the characteristic flavours are formed. The roast grade immediately after the end of first crack is called a City roast. The City roast is a light roast, and will still have a grassy flavour to it. The next roast grade is called City+, it happens about halfway through the second phase. Full City is a medium roast grade and comes after City+ roast grade. It is coffee that has been roasted to just before second crack. Full City+ roast happens just after the first snaps of second crack have occurred. City+ and Full City+ are the degrees that are usually considered good drinkable coffee. [37] Coffee roasted beyond the first snaps of second crack starts to get burnt flavours and is considered less desirable.

3.4 Roasting Technology

For roasting to happen, all that is required is the application of heat to coffee. Coffee is usually agitated to ensure that the coffee is evenly roasted. As the mechanical process for roasting coffee is simple, there are many ways of roasting coffee. Illy et al. [6] and Clarke et al. [32] list some popular methods.

Use of a rotating cylinder; a common method of roasting that involves placing the coffee in a rotating drum and heating the coffee by hot air pumped through either the centre of the cylinder or through its perforated sides (Figure 10). This roasting system is used in both batch and continuous roasting systems. A batch roaster holds the coffee in the roasting chamber then discharges the coffee into a separate cooler. In continuous roasting the beans travel through the roaster on a screw drive. In some rotating cylinder designs the chamber includes a cooling section before discharge.

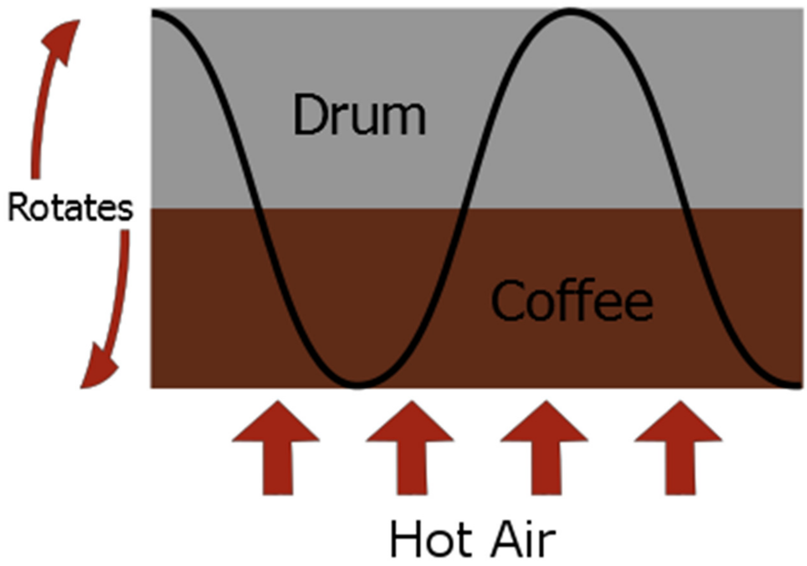


Figure 10. Diagram of a drum coffee roaster, low speed hot air is blown through the bottom of the drum. The drum rotates, moving the beans, ensuring an even roast.

The bowl method is an industrial method of coffee roasting that involves roasting the coffee in a rotating bowl. The coffee is pushed up the sides of the bowl by a combination of centrifugal force and hot air. When the roast is completed the coffee is discharged out the top of the bowl. The fixed drum (Figure 11) is another industrial method where coffee is placed in a vertical drum with rotating paddles. Hot air is blown in the bottom of the drum while the coffee is agitated using paddles.

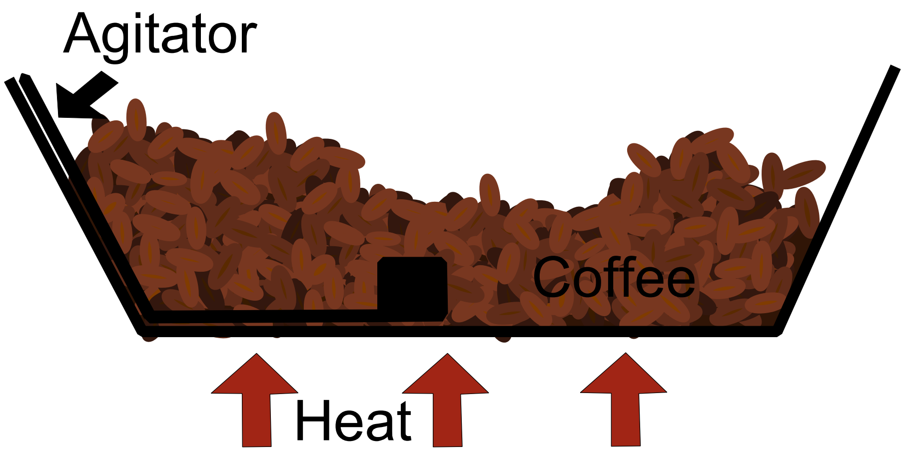


Figure 11. Diagram of a fixed drum coffee roaster. The drum is heated from the bottom while the coffee is agitated to ensure an even roast.

The fluid bed is a method of roasting that involves using heated gasses to fluidise[1] coffee acting as the agitation and ensuring an even roast (Figure 12). Fluidisation can be achieved by either blasting air from below or above the coffee. Fluidised beds are capable of the fastest roasting times as the convective heating from the air bed is a more efficient method of heat transfer. This method of roasting is also the easiest to measure and log data such as temperature and colour [32] and will be the base of this thesis.

The spouted bed is a variation on the fluidised bed. The coffee is forced up in a spout of hot air then falls to the side of the spout. This is easier to build than a full fluidised bed but produces a less even roast.[32]

The swirling bed is another version of the fluidised bed however the air is injected from the sides of the roasting chamber in a way to cause the air, and thus the beans, to spiral around the chamber.

[1] Fluidisation: is the process of blowing air though a particulate solid so that it behaves like a fluid.

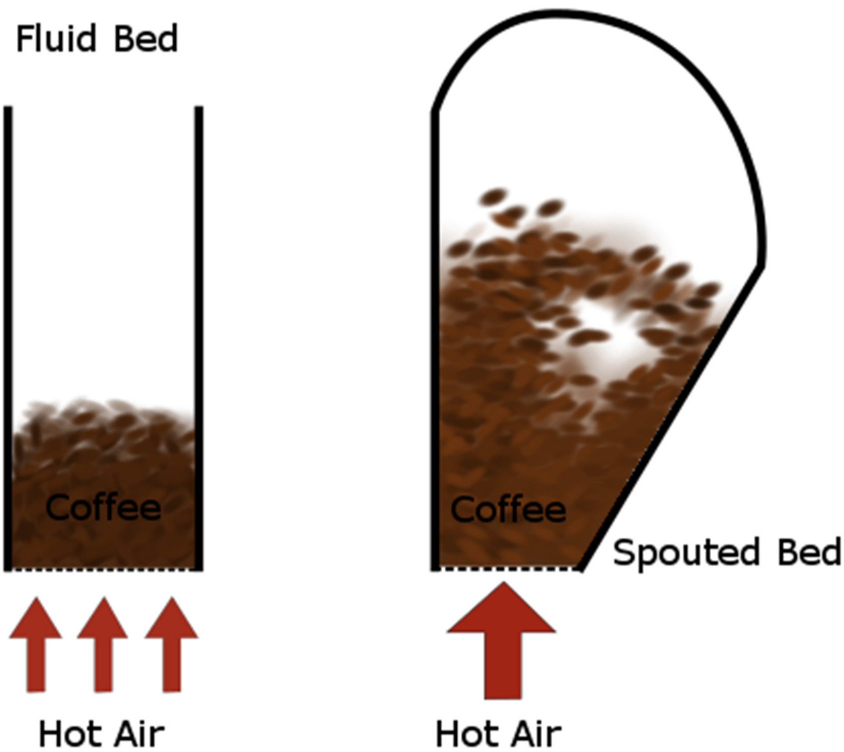


Figure 12. Diagram of fluid-bed (left) and spouted-bed (right) coffee roasters. High speed hot air is blown through the coffee simultaneously agitating and roasting the coffee.

3.5 Influential Works

This thesis takes guidance and inspiration from many different pieces of literature. This section looks at the pieces of literature whose content is directly applicable to this work.

The best place to start is the books on coffee by Clarke and Illy. Already referenced in this thesis, these books exist as a collation and summary of coffee roasting technology. Clarke's books *Coffee Volume 2: Technology (1987)* [5] and *Coffee: recent developments 2001* [32] are excellent collections of the knowledge and technology related to the production and processing of coffee. Similarly, Illy's book *Espresso Coffee 1st edition: the chemistry of quality (1995)*[38], *2nd edition (2005) : the science of quality* [6] provides an excellent summary of the science and technology taking coffee from cherry to espresso cup. A large portion of coffee roasting literature cite one or both these books.

Schenker's PhD thesis: *Investigations into hot air roasting of coffee beans* [1] looks at how the fluid bed coffee roasting of coffee affects the physical and chemical characteristics of the roasted coffee beans. The crux of Schenker's work is developing a method to understand how changing the roasting technique affects the flavour of coffee. Schenker's work involves comparing coffees after fluid bed laboratory roasting and drum commercial roasting. Part of the conclusion states:

> "Roasting technology cannot make up for poor quality of the raw material. However, for a given type of green coffee blend, roasting is the main flavour determinant."

Schenker's later work [39] looks at how changing temperature roasting profile affects aroma development. Looking at Schenker's works in relation to this thesis, Schenker highlights the effect that roasting has on the flavour of coffee as well as provide insight into the use of a fluid bed for coffee roasting.

Hernández et al's paper *On-line Quality Estimation for the Coffee Batch Roasting (2007)* [17] is a body of work looking at the use of visual sensors and modelling in roasting process control. In this paper, the author proposes a method of coffee quality estimation based on grayscale visual inspection of coffee beans. The tests run in this paper are on a single origin of coffee roasted in a very stable environment with uniform lighting. The paper then looks at using visual inspection to identify the temperature conditions of the coffee beans.

In Franca et al's paper *A preliminary evaluation of the effect of processing temperature on coffee roasting degree assessment (2009)* [16] small batches of single origin coffee were roasted to varying degrees at different oven temperatures. Numerous tests were run on the roasted coffee beans. The result of the study found that colour and mass loss alone were not a reliable method of degree of roast determination and that processing temperature was an important factor. This idea echoes Schenker's work on aroma formation [39].

An important aspect of understanding coffee is to understand what the average coffee roaster is looking for when roasting coffee. Looking outside the science and moving into a more subjective side of coffee brings us to Sweet Maria's and their visual guide to coffee roasting [40]. Sweet Maria's is one of many coffee roasting enthusiast websites. What makes it notable is the collection of roasting resources from the layman's coffee roasting perspective. Their online resources aligned with my experience of interviewing local roast masters. The cited page [40] contains a visual comparison of coffees at different degrees of roast and the roast masters opinions on whether the particular degree of roast is acceptable or drinkable.

3.6 In Search of the Ideal Degree of Roast

Roasting a perfect coffee for brewing is not a trivial task. A roaster requires a lot of experience at interpreting the changes and events that occur during coffee roasting to produce an ideal roast. The wide range of changes, colour, size, texture, roast chamber temperature, and elapsed time are all indicators used to help determine the ideal degree of roast.

There is research that considers many of these changes to help detect and define coffee's degree of roast. A commonly used technique is to look at bean colour during roast. Colour is often used to represent or display a particular degree of roast.[30], [36], [37] Colour sensing suffers from some drawbacks. First, the application of colour sensing in a calibrated and/or online setting is very challenging. Secondly, coffee roasted to the same degree of roast using colour as the measure will not always have reached the same degree of roast in terms of chemistry. The consensus is that colour is not repeatable enough to reliably predict the degree of roast.[41]

Some authors have looked at determining the degree of roast by looking at the roaster exhaust gas[2].[33], [34] Mass spectrometry has been used to identify the compounds in the exhaust but is not often able to work in real time. Real time mass spectrometry has been investigated using laser ionization mass spectrometry.[34] Gas chromatography has also been used to measure the exhaust gas compositions.[15] Each of these techniques had varying success in identifying the various compounds produced in a roast. None of these techniques has led to a reliable method of measuring degree of roast, likely due to cost and/or lack of real time applicability.

Sound has also been used to monitor roast progression. P. Wilson [42] used sound to detect the notable pops at first and second crack. P. Wilson found that the sounds of the cracks are both detectable and distinct from each other. The detection of the cracks using sound is interesting and would work for any roast that was to end after second crack. However, after looking at Sweet Maria's roasting chart and discussing with people who roast coffee, most acceptable roasts occur before second crack. If the goal of the person roasting the coffee was for a roast lighter than Full City+ [40] (fractionally after second crack) a sound based system would be pointless.

Temperature is often used as a method of roast control as it is straightforward to measure and report. Temperature has been suggested as an indicator for the determination of degree of roast.[43][44] It is well accepted that temperature does affect the resulting coffee. However, it is not a perfect measure of degree of roast as a roast's temperature profile is also known to affect the final coffee.[6] There is merit in the measurement of temperature to determine degree of roast but it will have to be done differently than it has been done before.

The goal of this thesis is to help determine a method of detecting an ideal degree of roast. Considering the broadness of the topic this is obviously a very subjective goal. Therefore, the target was refined to creating a method of predicting second

[2] Many expert roasters do without access to the exhaust gas from the roaster. In most industrial and commercial settings, the pervasive smell produced by the roaster is ducted away from the roaster.

crack using a previously undetected transient. The benefit of such a method would be that it could be used independent of the origin of the coffee.

To this end this thesis looks at different sensor types to track online changes in the coffee as it roasts. The tested methods were to: observe the coffee's changing heating characteristics; observe the coffee's changing permittivity and hence moisture loss; and observe changes in the coffee's surface chemistry using Raman spectrometry spectroscopy. As well as the sensory techniques that were tested, research into different techniques that were plausibly useful, but were not testable, was done.

3.7 Researched Approaches that were not Possible to Test

3.7.1 Thermal Imaging

There is no record of anybody pointing a thermographic camera at coffee beans while they roast. It turns out that this is for good reason. Investigations into this technique found that it was not as straightforward as it might seem.

What is thermographic imaging? More commonly referred to as thermal imaging it is a method of producing an image where the pixel value is a measure of temperature. Thermographic cameras can measure the infrared black body radiation coming off an object and convert it into a pixel value.

The problem faced when trying to thermal image roasting coffee is that the coffee is inside a coffee roaster. For the most part coffee roasting machines have very little visual access but in the rare cases where the coffee is visible the infrared radiation is blocked by various mediums.

Regular glass blocks the passage of infrared in the range that thermographic cameras work[3]. This means that although a human observer could watch the coffee the thermal camera would only see the heat from the glass. This makes observing roasting coffee with a thermal camera tricky. A possible method of making it work

[3] Glass typically Silica or Quartz has an upper frequency transmission limit around 4µm [45]. Thermal imaging cameras start operating around 7µm [46].

would be to add a window to the side of the roast chamber made of a material that would let the infra-red pass.

There are a few problems with adding a window the biggest of which is what material to make it out of. There are quite a variety of materials that allow the transmission of the infra-red, however most are not suitable for coffee roasting. Polyethylene for example[47] allows the infra-red transmission in the desired frequency range but would melt at the temperatures reached by the coffee roaster. Potassium chloride is another candidate[45]. However, because it is a salt it means it is also water soluble. This becomes problem in an environment with a large amount of moisture — such as in the exhaust gas of a coffee roaster. Another option was diamond, although this has the obvious drawback of being very expensive.

If a suitable window was located, it would require a heavily modified roasting chamber to fit the window. In the end, although possible, it was going to be too large an exercise to make it worth to taking a measurement.

3.7.2 Headspace Analysis

Headspace chemical analysis is a very promising approach. The basic idea is to measure the chemical composition of the exhaust gas to give a good impression of roast progression. Several different approaches were considered: Full chemical analysis, the construction of an electronic-nose, and the use of flame or photo ionisation detection to measure bulk flammable volatiles.

3.7.2.1 Chemical analysis

The first option is to apply a method that would do a full chemical analysis of the head space gasses in the exhaust. This approach has been done before and has produced promising results. However, the methods used to take this type of measurement are either an extensively offline process or require expensive equipment. [33], [34]

There was a plan for doing this method with a spectrometer (ideally the Raman). The problem was in the execution; in the case of Raman, the amount of Raman scattered light that comes off particles of gas is prohibitively small. To get enough Raman scattered light back to the sensor would require many interactions between laser and gas. The two ways to do this are either a very long exposure time (not possible online) or a long path length cell.

A long path length cell is a cell where the spectrometer's laser is reflected between mirrors so that it passes through the gas in the cell multiple times. A long path length cell is a theoretically possible addition to the test coffee roaster constructed for this thesis. However, it would have required a custom optical setup. This made it impractical for the tests in this thesis.

3.7.2.2 The Electronic-nose

Another option for head space analysis would be to use readily available chemical detectors. Such a setup has been used to tell the difference between two types of green coffee [48]. However, it also has pitfalls.

There were two major problems with this approach. The first, it was not clear what compounds would be important. These sensors are designed to find very specific chemicals and there was no guarantee that the available sensors would be able to detect useful chemicals. The second problem was temperature. These sensors are designed to work at room temperature. It is not uncommon for them to have rated temperature limits around 50°C. This is a real problem when you are trying to measure +200°C air. In the end this method was not going to be practical.

3.7.2.3 Flame (and Photo) Ionization and SIFT-MS

Lastly there exists a method of measuring bulk volatiles coming off a sample's head space: Flame Ionization Detection (FID). FID works by passing the sample through a hydrogen flame. The flame is held between a pair of capacitive plates. As the sample burns in the flame the current passing between the plates changes. The larger the amount of sample burned the bigger the change in current. Similarly, Photo Ionization Detection (PID) works by ionizing the sample using high energy light and then, similarly, the ionized sample is passed through capacitive plates. These methods can show how much material is passing though the sensor but not its composition. Additionally, they are relatively inexpensive to implement— at the time of writing a PID sensor cost around USD 800. It is not clear however, if a non-discriminatory measurement of the volatile gases produced during coffee roasting hold enough information to be helpful.

During the writing of this thesis the technology SIFT-MS (Selected ion flow tube mass spectrometry) was identified as a method that would help answer this question. A literature search for the use of SIFT-MS on coffee roasting turned up nothing. However, "Syft Technologies", a manufacturer of SIFT-MS devices, published the results of its application to coffee roasting on their website[49]. Their results show gradual progression in the amounts of measured volatiles for all points except first and second crack. This would mean that a non-discriminatory method such as FID would not detect a second crack precursor.

3.8 Contextual Summary of Tested Measurement Approaches

The methods that were chosen for experiential evaluation were, thermal analysis, microwave aquametry, and Raman spectroscopy. The goal in choosing these test methods were:

a) They had not been tried previously in a coffee roasting context
b) They were hypothetically able to be reduced to a level that could be added to a consumer grade device
c) They were able to give some insight to the condition of the roasting coffee

"When looking for green frogs you pick up anything that is green" – J. Scott (2017)

Thermal analysis was chosen for its simplicity. There are various accounts of coffee's changing thermal behaviour; however, the question remains, can it be used as a method of roast control? Additionally, is there a way to use a thermal measurement method that would get more information than in standard practice while still roasting the coffee? A fluid bed coffee roaster was constructed for this work so that different heating profiles could be tested.

Microwave resonance quality measurements of coffee were chosen for their uniqueness. The moisture level of the coffee is known to change dramatically during coffee roasting. This alone has a significant effect on the permittivity of the coffee. If the rate of moisture loss in the coffee is not linear it may lead to an unknown transient or waypoint that can be used in the prediction of second crack.

Finally, Raman spectroscopy was chosen to allow for the observation of the coffee's changing surface chemistry. The change in the coffee's colour, and therefore chemistry, is one of the most obvious changes in coffee as it roasts. The Raman spectrometer gives the flexibility to measure the coffee's changing surface chemistry during online roasting.

4 A Thermal Study of Coffee Roasting in a Fluidised Bed Coffee Roaster

4.1 Chapter Introduction

This chapter covers the design and construction of a fluidised bed coffee roaster. The temperature measurements taken from the coffee roaster are done using various thermocouples. The thermocouple measurements were logged and used for temperature control. Using a fluidised bed enabled control of the air temperature around the coffee; allowing the testing of roast profiles uncommon in literature.

The chapter then moves on to testing a method of observing thermal changes in the coffee. The major benefit of temperature sensing is its convenience. Direct measurement of the coffee produced results no different from what is reported in other literature. Use of a ramp profile —which is different from that which is found in most literature[43] — was able to produce a unique result by allowing for a method of qualitative calorimetry. This was done by considering the idea of "bean load". The bean load is a representation of the energy absorbed, or produced, by the coffee during roasting. This is similar to how an unknown load would be treated in an electronic circuit.

The result of bean load measurements showed a significant loss in energy caused by the evaporation of water in the early roast. What happens after this is initially less obvious but there appeared to be a distortion created during first crack. Comparing the distorted result to later results made the distortion look exothermic (which is unexpected due to the nature of first crack). To gain a better understanding of the system a model matching the thermal behaviour was created in SPICE (Simulation Program with Integrated Circuit Emphasis).

The SPICE model matched the coffee's behaviour in terms of thermal capacity and energy lost to the evaporation of moisture. The model and measured results showed a more exothermic dip in bean load pre-first crack as evaporation of moisture was lessening. Once first crack is reached the model and measured results start to disagree. During first crack, the measured signal becomes more endothermic than the model.

Due to limitations in the experimental coffee roaster this thermal measurement method was not able to measure all the way to second crack. However, comparing the post-first crack measurement to the model there are no more obvious deviations. Also, the signal to noise ratio is small meaning it is unlikely that chemical thermal reactions will be measurable using this method. Although the results were interesting, they were ultimately unhelpful.

4.2 Building a Coffee Roaster

To study coffee roasting in detail, a coffee roaster was constructed which was used to run roasting experiments. The roaster needed the ability to have various sensors attached and have temperature and airflow rate controlled with fine detail. To this end, a fluid bed coffee roaster (Figure 13) was chosen. As discussed in the previous chapter, roasting is achieved in a fluidised bed roaster by blowing hot air through the beans. The fluidised bed allowed for the control of the air temperature and flow rate of the air that passed through the coffee beans.

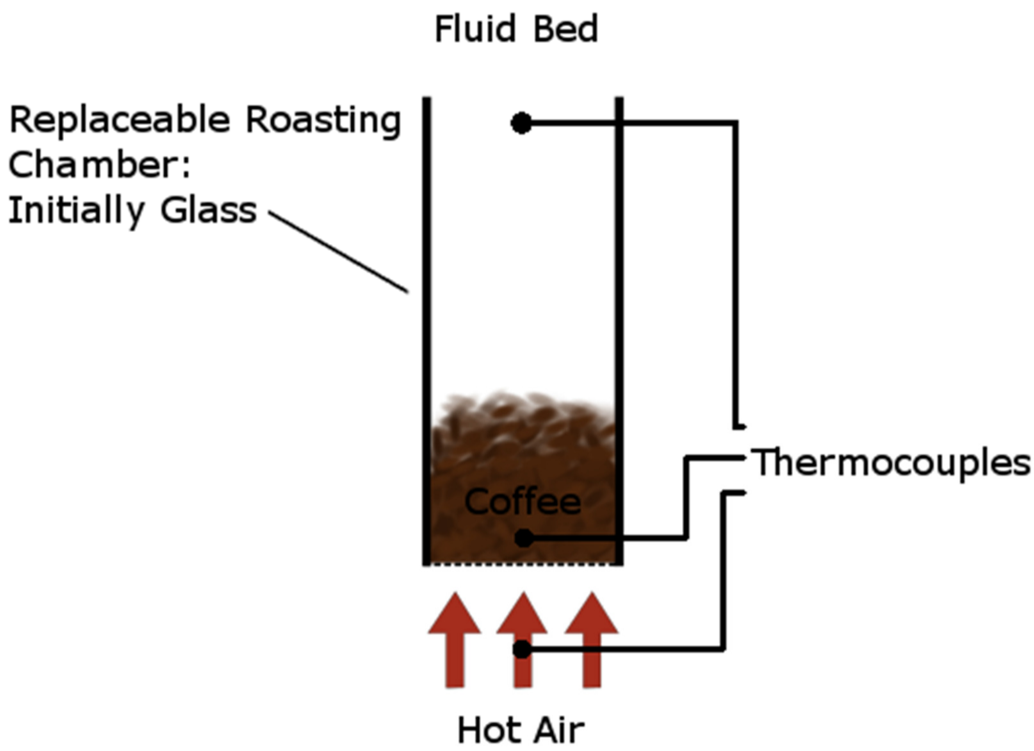


Figure 13. Initial conceptual design diagram of the fluid-bed coffee roaster.

4.2.1 Original Design

The original coffee roaster design was based off a popular small-scale roaster design made by modifying a popcorn popper (Figure 14). The popcorn popper blows hot air into the base of a small metal chamber causing the grain to swirl. Unfortunately, the stock popcorn popper did not get hot enough to correctly roast the coffee. The coffee roaster had to undergo a major redesign as the popcorn popper was not controllable and could not hold up to the required modifications.

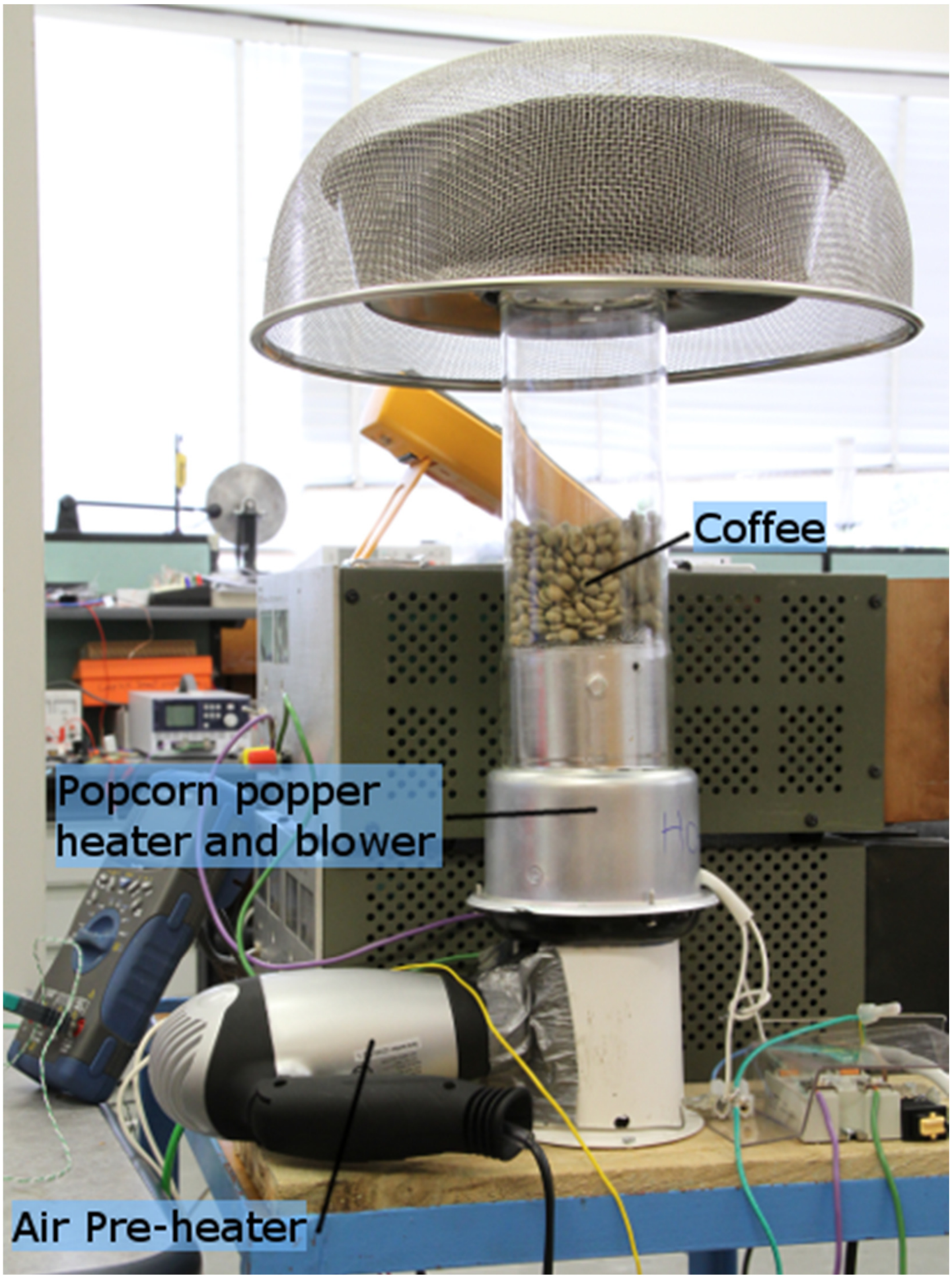


Figure 14. Original coffee roaster design. Based on popcorn popper. It could roast coffee but unreliably.

4.2.2 Redesign

The roaster was redesigned to allow improved control of both temperature and air flow. The rebuilt roaster also allowed for the use of more rigorous parts that would work better under the test conditions. The roaster was mounted to a display board for easy access and manoeuvrability (Figure 15). This configuration permitted the mounting and affixing of the various sensors and control electronics the roaster needed.

The roaster consists of a roast chamber that holds the coffee during that roast. This chamber is connected to a heating element that heats the air. The element is in turn connected to a blower that blows air through the system. The heating element and blower are both connected to a measurement interface so that they can be controlled by a computer.

4.2.2.1 Heating Element and Blower

The heating element was taken from a heat gun. The heat gun was rated on its packaging to 2000W[4]. This rating was not tested. However, it was sufficient for the coffee to reach roasting temperatures.

A few blower configurations were tested in the design. An industrial blower that came with a built-in control mechanism was included in the final design. This blower was suitable to fluidise around 140g of green beans on its highest setting.

4.2.2.2 Roast Chamber

My main roasting chamber was made of glass (Figure 16). Glass was chosen so that the coffee could be easily observed throughout the roast. This was a good idea in theory and did allow for easy setup; however, the heat loss through the glass sides of the roaster was significant and could skew the measurements. For that reason, during most tests, the roaster was wrapped in a sheet of fiberglass insulation.

[4] This value was likely reached as a function of the heating coil's resistance. The coil had a resistance around 30Ω assuming an RMS mains voltage of 240V works out to be 1920W or the roughly 2kW.

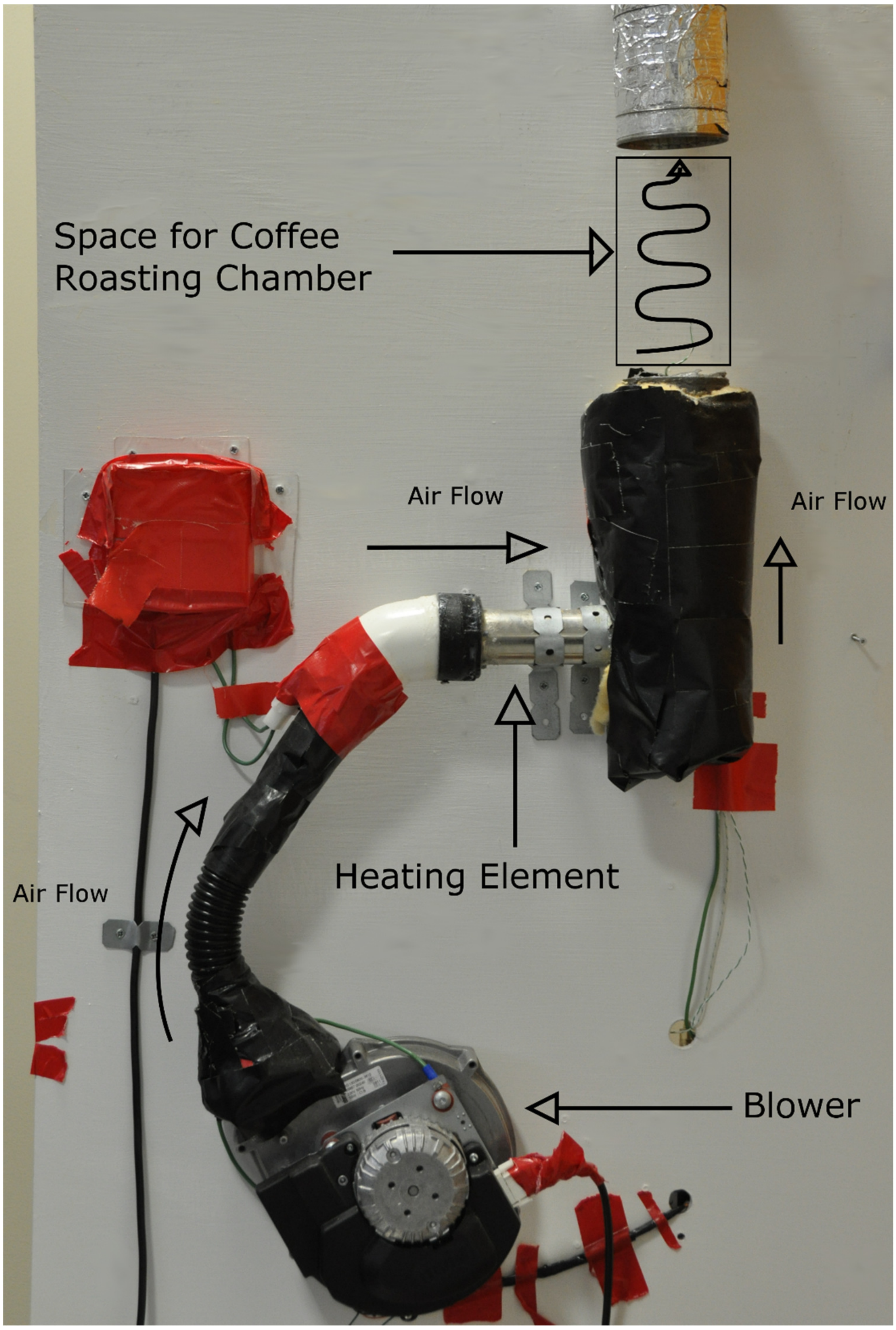


Figure 15. Redesigned and built Coffee Roaster. In this figure, the roasting chamber has been removed. This design was more reliable and allowed for the roasting chamber to be replaced.

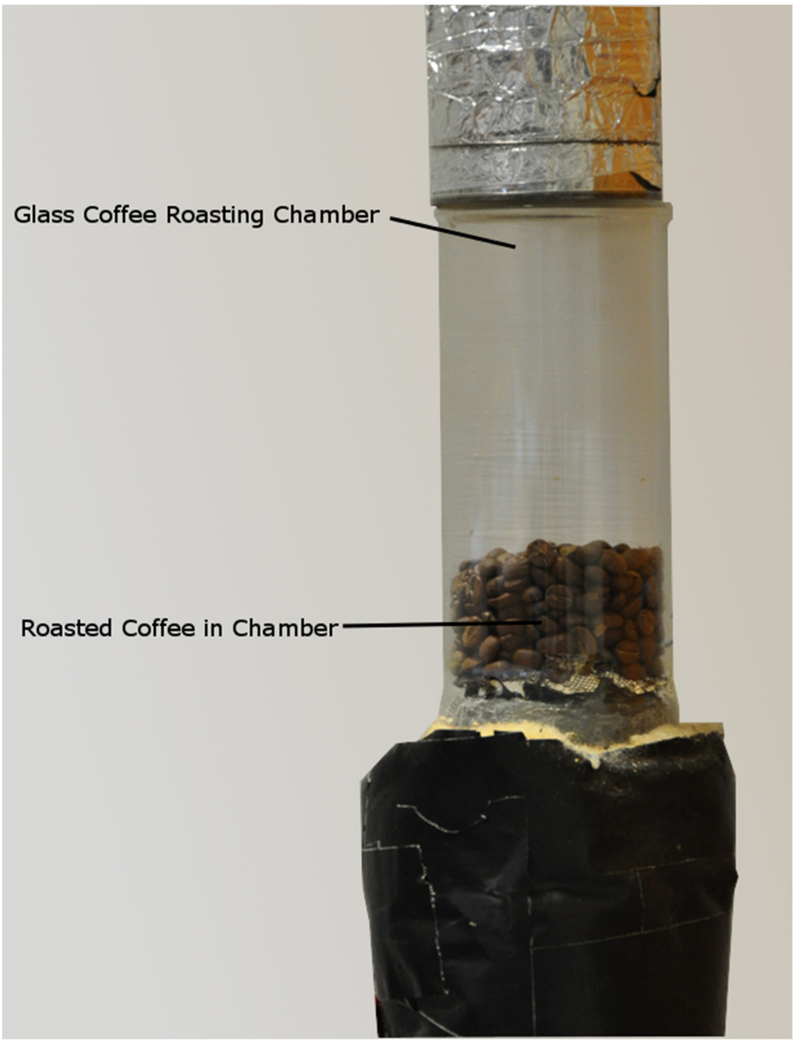


Figure 16. Glass roasting chamber with roasted coffee.

The roaster's control was run on a computer. The computer was linked to the roaster by a Labjack measurement interface.[50] The Labjack allowed for a simple communication method between the roaster and the control computer. Figure 17 contains a basic layout of the roaster and control system. A full layout diagram is included in the appendix.

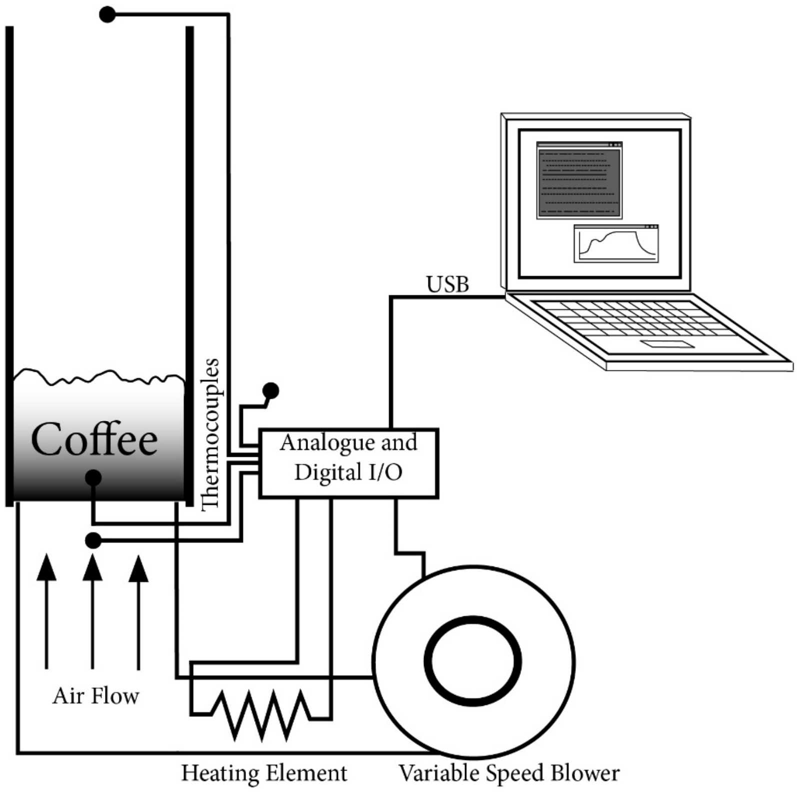


Figure 17. Functional diagram of the coffee roaster. Air is blown through the heating element and into the coffee. Thermocouples linked to a computer logged the air temperature at the input to the roast chamber, inside the coffee, and at the exhaust of the roast chamber. The computer was used to log and control the roast air temperature.

4.2.3 Temperature Measurement and Control

Temperature measurements were made using several thermocouples placed strategically on the roaster. The thermocouples used were K-Type thermocouples that were each connected to a thermocouple amplifier [42]. The thermocouple amplifier measures the thermocouple's analogue signal, then calibrates and amplifies it. The analogue signal's value is proportional to temperature. The outputs of the amplifiers were then connected to the Labjack.

A closed loop PID (Proportional-Integral-Derivative) control system was written which was intended to control the temperature of the air at its point of contact with the beans. The control was applied to a thermocouple that was set in the beans.

Temperature measurement is often used in roaster control as it is straightforward to measure and report. Additionally, the temperature is linked to the chemical reactions that happen in the coffee. The exact temperature that is measured is dependent on the roaster and where the temperature sensors are located; meaning that a temperature result is not necessarily transferable from roaster to roaster.

It is well accepted that the roast temperature does affect the final roast.[6] Moreover the temperature profile of a coffee roast can affect the quality of the coffee produced.[16] A roasting coffee bean's temperature has been suggested as an indicator of the degree of roast.[12][16] Most of the literature uses a "step" temperature profile that has the roasting environment at a fixed target temperature. The "step" profile simulates the temperature profile that coffee would experience in a drum roaster — a common commercial roaster.[29][44]

Using a fluidised bed roaster —for which precise temperature control was possible—meant that a different temperature profile than the standard "step" profile could be used. The PID control loop was used to apply a fixed linear temperature ramp to the coffee — unusual in literature. The "ramp" profile gave a sensitive view of the coffee's thermal effect on the environment. The idea was that by observing the temperatures and temperature changes the coffee's progression could be tracked through the roast.

The "step" profile (Figure 18) replicates adding the coffee into a roaster that has been preheated to a target temperature. The coffee's temperature rapidly goes from room temperature to the target temperature and stays there until the roast is completed. The "ramp" profile (Figure 19) started at room temperature and then slowly increased the temperature until it reached a target temperature late in the roast.

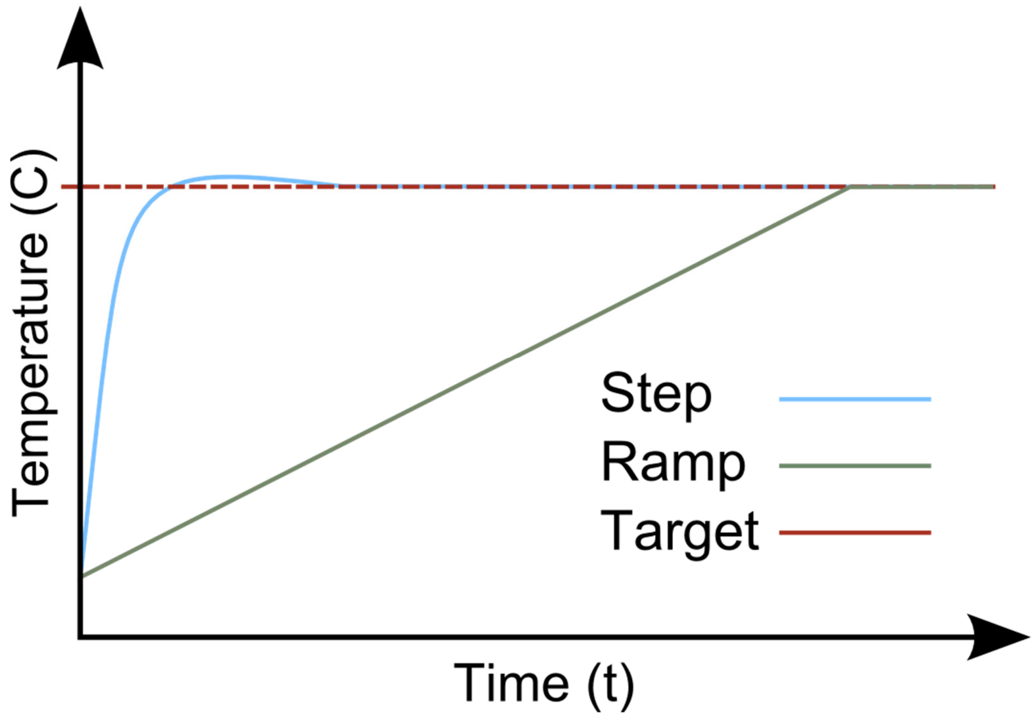


Figure 18. Comparison of different temperature profiles. The step profile is the standard coffee roasting profile.

4.3 Ramp Roasting Coffee

My initial test used 67 ± 2g of a green Costa Rican Arabica coffee. This volume of coffee was the same as that used in the original popcorn popper design and was chosen as it fluidised well producing an even roast. Several ramp gradients of 0.06°C/s, 0.07°C/s, and 0.08°C/s were tried (Figure 19). Each roast started at room temperature and ramped until the target temperature of 240°C. The target temperature was chosen as being near the limit of reliable control available to the roaster.

The plots in Figure 19 show the temperature results from roasts of different ramp values. The plot shows the three roaster thermocouples' readouts, the highest temperature trace denotes the input air temperature, the middle trace represents the thermocouple situated in the coffee, and the lowest trace plots the exhaust temperature. The "in coffee" thermocouple — that measures the air temperature at the surface of the coffee — was used as the control input.

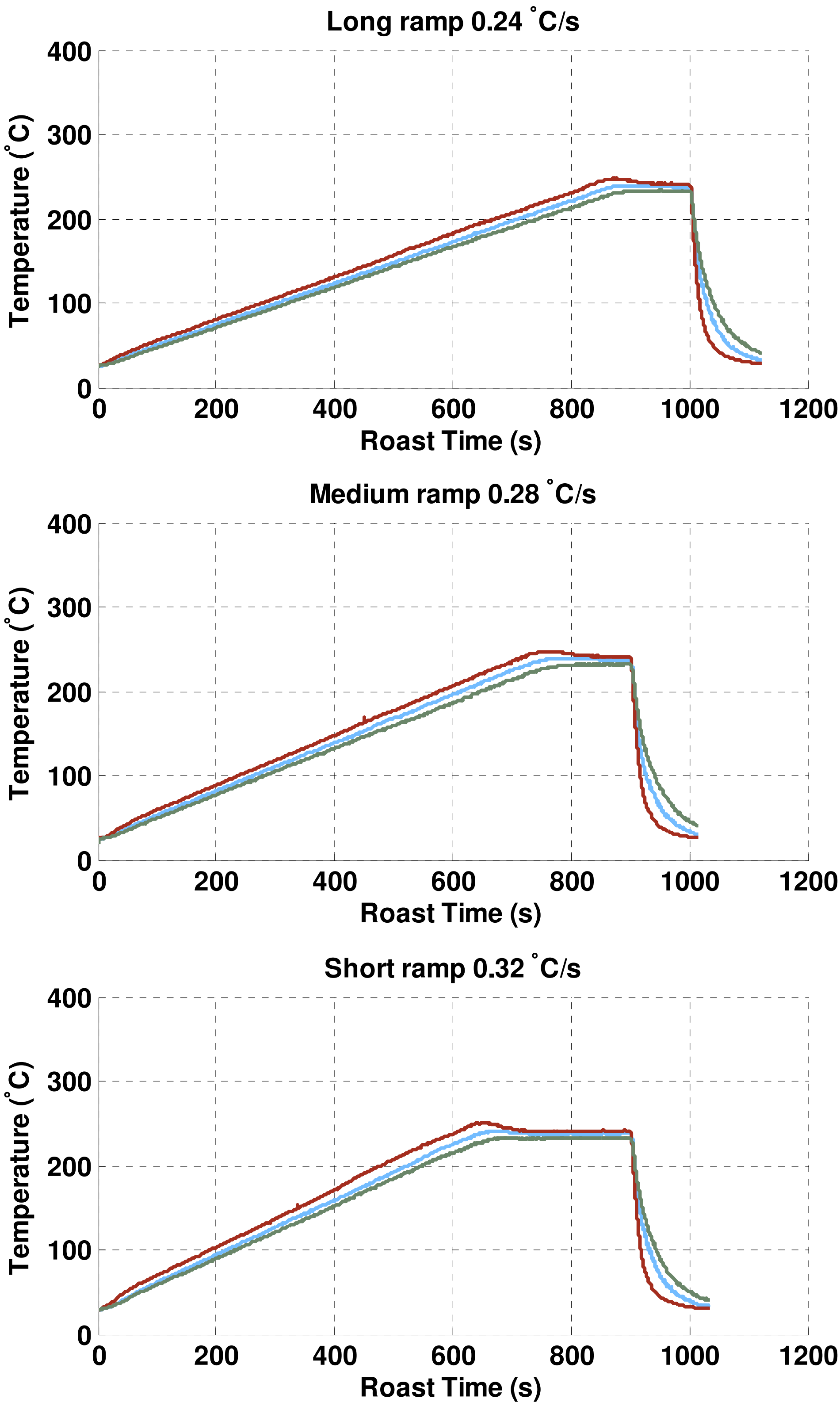


Figure 19. Different temperature ramps for a target temperature of 240°C; red – input temperature, blue – coffee temperature, green – exhaust temperature.

4.3.1 Looking for Changes in Control Output

The first area examined was the control output power. The idea being that the changes in the thermal properties of the coffee (over the course of the roast) would cause the control system to require varying amounts of power for the heater to maintain the ramp.

Figure 20 displays the control input, the control output, and the coffee thermocouple temperature. The control input was calculated as the difference between the target temperature and the measured temperature. The control output was the Pulse Width Modulation (PWM) percentage that was sent to the solid-state relay which controlled the heating element. Unfortunately for the experiment, after looking at the results presented in the graphs, there did not seem to show any perturbations on the control input, control output, or the —for the control loop— measured temperature that would indicate the presence of any thermal effects from the coffee.

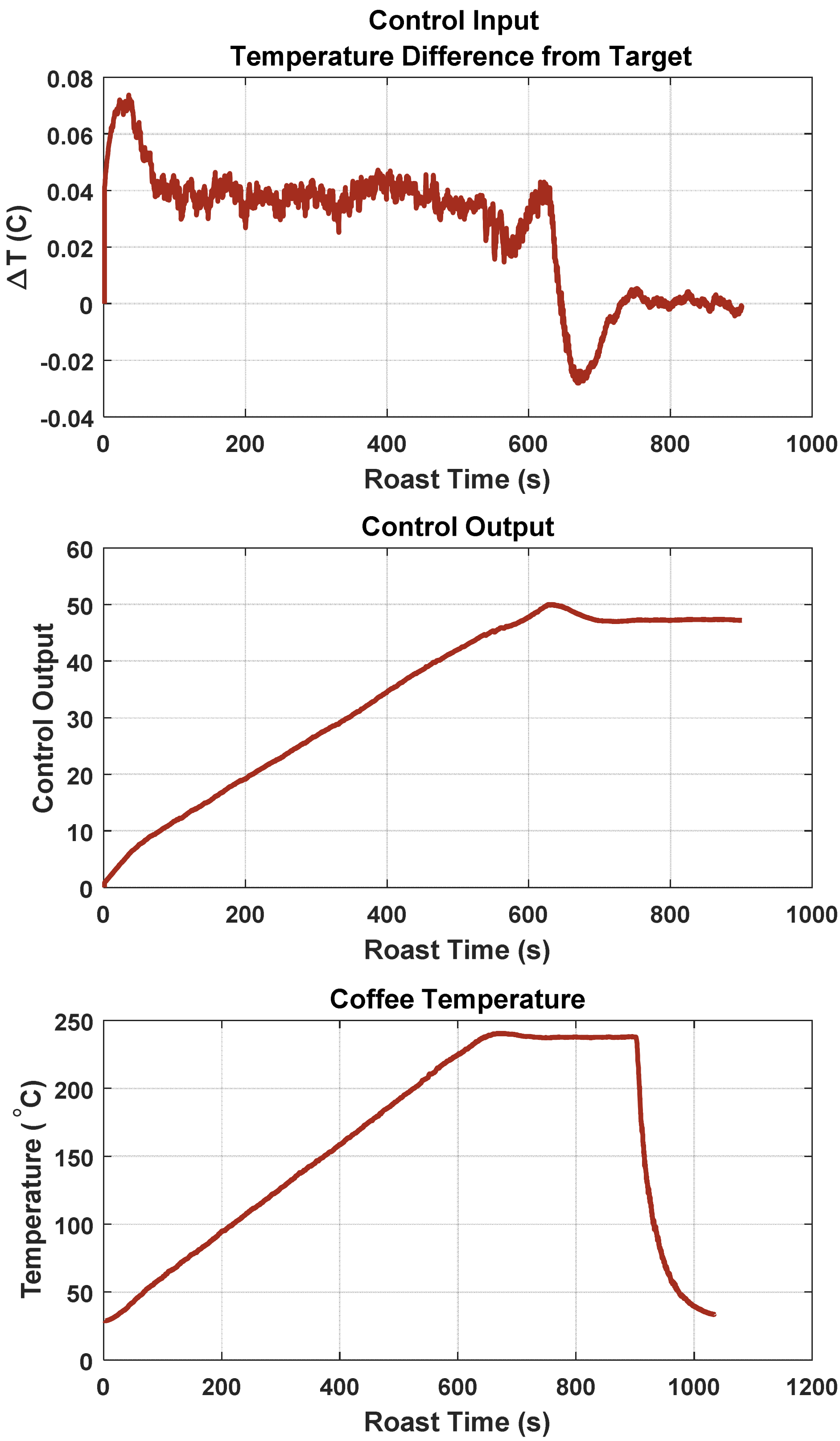


Figure 20. Showing the control input, output, and coffee temperature.

4.3.2 Looking for Changes in Input Output Temperature Difference

The second plan was to look at the difference from the input and output temperatures of the roasting chamber (ΔT). What should be seen is the load that the coffee places on the roaster. Any reactions occurring in the coffee during roasting would be reflected in this measurement. The difference plots from the three ramps tested are plotted in Figure 21 — the roasts are still using 67 ± 2g of coffee.

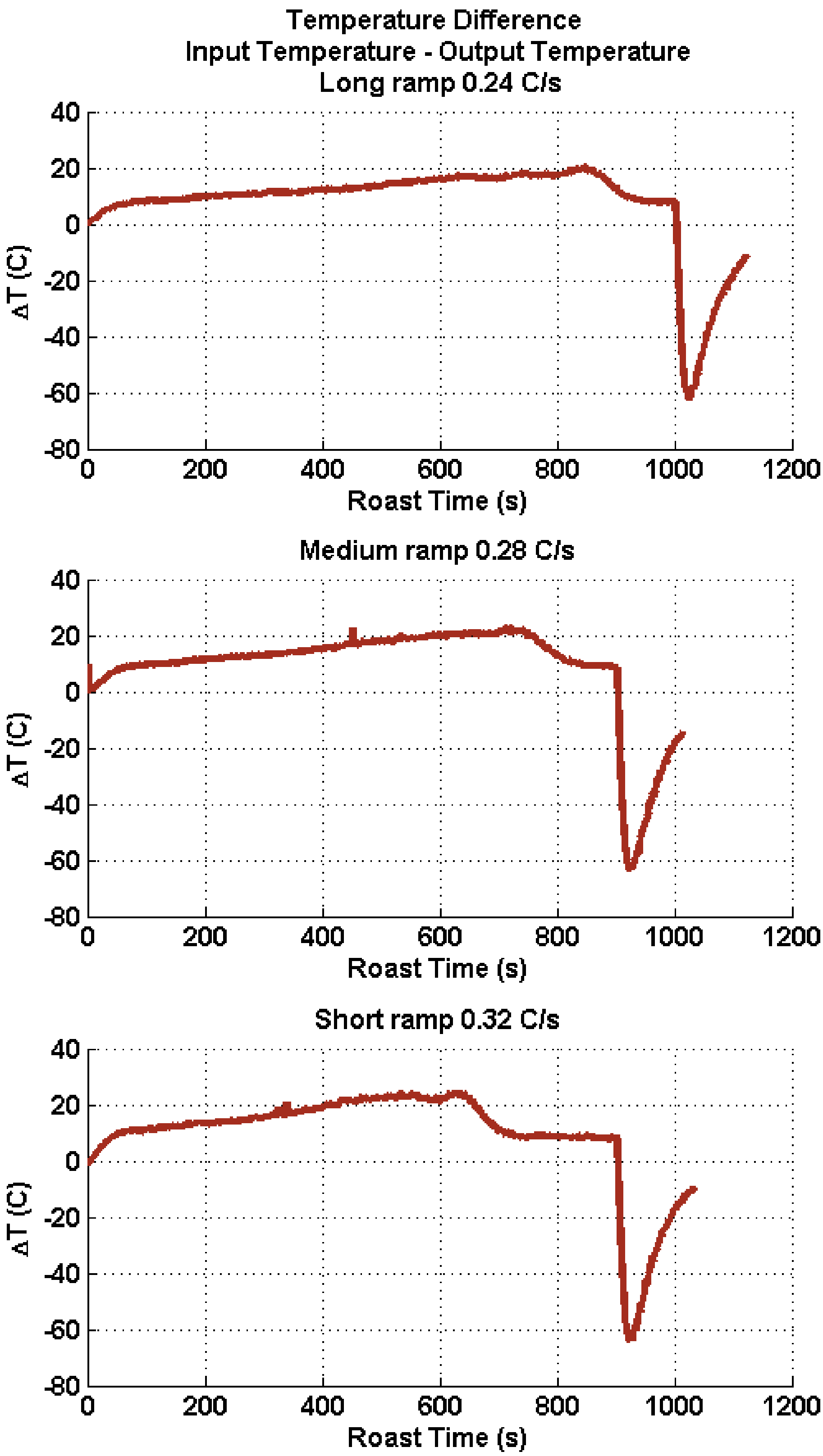


Figure 21. Shows the difference plots from the different ramp profiles.

Looking at Figure 22, the difference between the input and output temperatures increases as the roast progresses. The rate of increase lessens toward the end of the roast, around 550 s in the 0.28 °C/s ramp case. The expansion of the gap between the input and output temperatures was attributed to endothermic reactions in the coffee.

A limitation of this test was that the signal measured was rather weak and susceptible to noise. To increase the effective signal being seen, tests using a larger roast size —124 ± 2g were run. If the effect is related to the coffee beans' chemistry the larger roast size — double — should amplify it. The decision was made to run the roast with the 0.28 °C/s ramp which worked as a middle ground between maximising rise time — showing all the features of interest — and not taking too long to roast. These tests returned the expected larger load signal (Figure 22), which shows that the endothermic reactions in the coffee were causing the difference in input and output temperature.

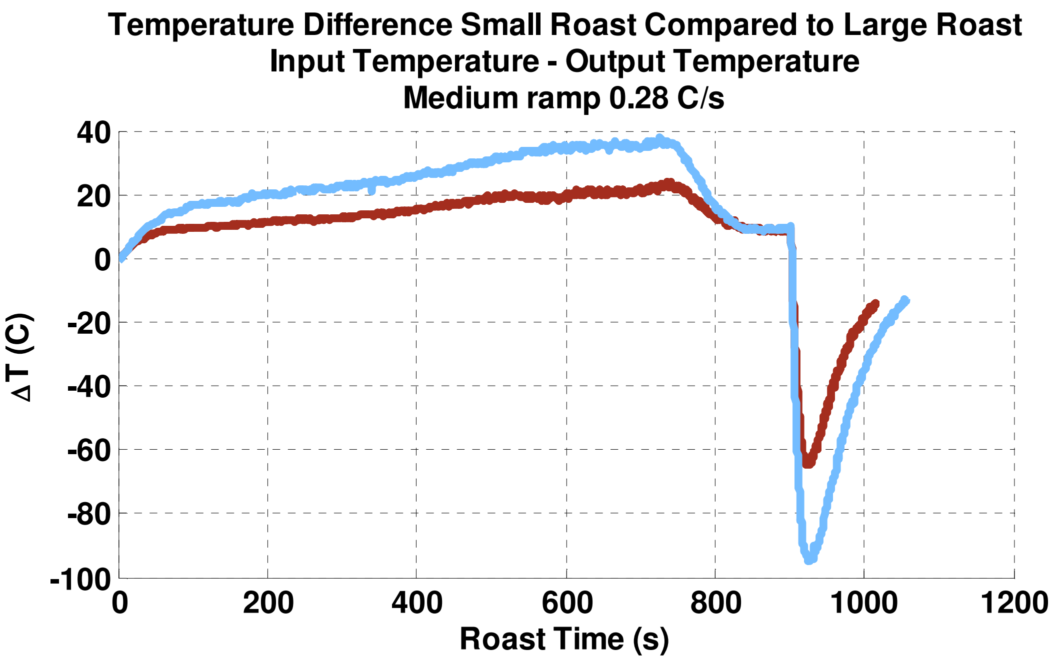


Figure 22. Single trace of the temperature difference from a large run (Blue) compared to a smaller run (Red). This shows that a larger mass of coffee increases the amplitude of temperature difference (ΔT).

4.4 Bean Load

4.4.1 Calorimetry

At this point it is important to consider the science of heat and energy exchange, Calorimetry. Calorimetry is the science and methods of measuring the heat exchanged in a system. It is used to determine heat transfer and the reactive heating or cooling of a sample. A machine used to measure the heat transfer is called a calorimeter.

The goal of a calorimeter is to account for all the energy in the system. These come in many forms, as there are many methods of measuring heat transfer. The calorimetric method chosen depends mostly on the sample and process under test.

The basic principles, some history, and some common calorimeter methods are outlined in the first chapter of "Calorimetry: Fundamentals and Practice"[52]. This chapter includes a description of one calorimeter design dating back to the 1700s. This design by Antoine Lavoisier was used to study respiration by measuring the body heat of a guinea pig. Another method mentioned is flow calorimetry. In flow calorimetry two flowing chemicals are mixed and the temperature of the chemical is measured before and after the mixing. Any thermal change caused by the mixing will be measured in the temperature difference.

Modern scientific calorimeters work on the same principles but go to great lengths to make sure that all aspects of heat flow and transformation are accounted for. A typical example of a modern calorimetry method is differential scanning calorimetry (DSC). In DSC, a sample is heated in a small pan next to an inert mass[5]. The temperature of the sample and the inert mass is measured. The difference between the two temperatures represent the amount of heat produced or lost by the test sample [53].

Calorimetry is a useful tool for understanding the thermal behaviour of substances. Its application to coffee roasting is apparent. The difficulty is applying calorimetry to batch roasting coffee online but this can be done by considering the heat flow through the coffee roaster. By accounting for the heat losses in the coffee roaster allows for the coffee roaster to be considered as a pseudo-calorimeter. The basic heat flow in the system (carried in by a flow of hot air) is depicted in Figure 23.

[5] Due to the physical size limitations of scientific calorimeters it is difficult to use them to make measurements on whole coffee beans. It is possible to make a measurement on coffee; however, it needs to be ground into a power. Therefore, such a measurement does not have much use because a lot of coffee roasting's defining characteristics come from the physical characteristics of the coffee bean. Despite this, the results of a DSC and thermal gravimetric analyzer measurements on a small sample of ground green coffee can be found in appendix 9.1.

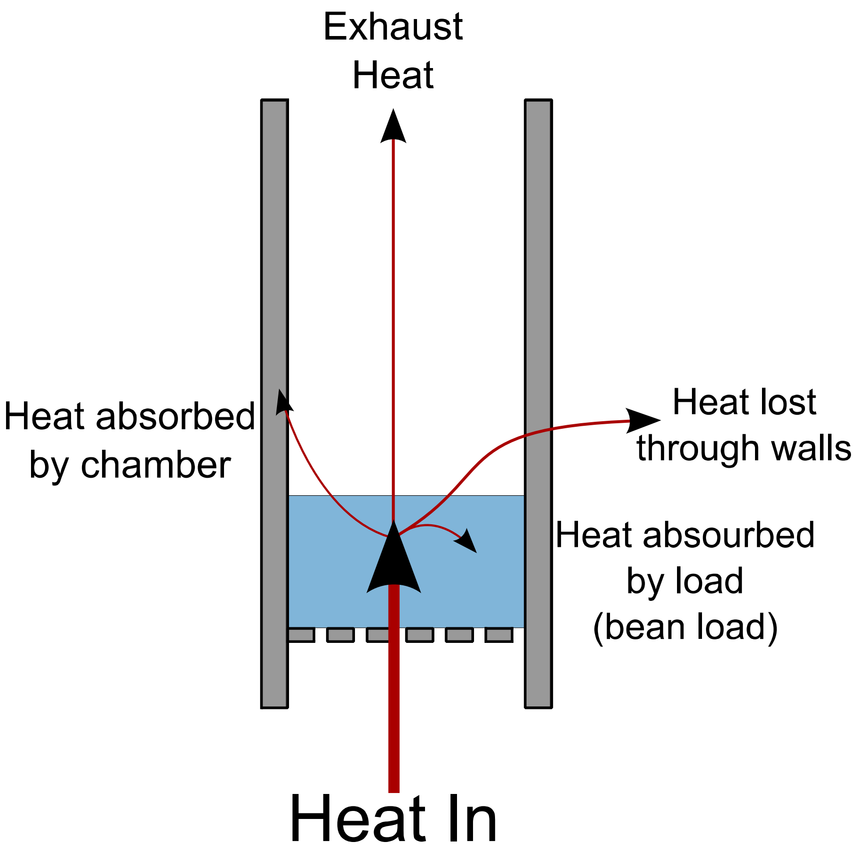


Figure 23. Heat flow through the coffee roasting chamber

A tool that can be used to help understand heat flow is to consider the system as an electronic circuit. Because the nature of heat flow and electric current flow are analogous, heat flow can be expressed as current flow in an electric circuit. This technique is quite common and other examples using this method to explain heat flow are included in F. Kreith et als', *Principles of Heat Transfer* [54].

This idea flows into Ohm's law and Newton's law of cooling being analogous. $V = I.R$ becomes $\Delta T = \dot{Q}.R$. Applying this analogy to the coffee leads to the qualitative concept of "bean load". The interest is in seeing how the beans absorb or produce energy during a roast. Treating the beans as a thermal load in a manner similar to an unknown electrical load, the energy lost and absorbed by the coffee can be represented in the same way as an electrical load. The bean load calculation is the difference of input to output temperature normalised against an empty run:

$$L_{bean} = \frac{(T_{in} - T_{out})}{\dot{Q}} - \frac{\left(T_{0_{in}} - T_{0_{out}}\right)}{\dot{Q}_0}$$

Where $\dot{Q}$ is the heat flow rate (which is proportional to the air flow rate at constant pressure[6]), T_{in} is the input air temperature measured beneath the roasting chamber. T_{out} is the air temperature at the exhaust of the roasting chamber. $\dot{Q}_0$, $T_{0_{in}}$ and $T_{0_{out}}$ are the same for the case of an empty roast chamber.[7] In effect L_{bean} represents the energy absorbed by the beans (i.e. the load on the roasting chamber).

The values used for the empty roast case were created from the average of multiple empty runs (Figure 24).

$$L_0 = \frac{(T_{0_{in}} - T_{0_{out}})}{\dot{Q}_0}$$

The normalising step, subtracting L_0 from the load of a coffee roast, accounts for the energy absorbed by and lost out the side of the chamber, which means that the result is comparable to a method of calorimetry. It shares elements with DSC and flow calorimetry[8].

4.4.2 Inert Bean Load

Applying the bean calculation formula to measurements taken using glass marbles in place of coffee beans produced the results in Figure 24. The marbles act as an inert load because their heat capacity remains constant for the duration of the roast. The values of inert bean load plotted in Figure 24 have been passed through a 50-point wide (roughly 1.5% of the total roast length) 4 Hz median filter. The marble load — after an initial ramp as it reaches an equilibrium — holds steady (varying less than plus or minus a quarter of a unit) during the roast's ramp. This result is consistent with what is expected from an inert load.

---

[6] Derivation of this in appendix 9.3

[7] In all my roasts I assume the air flow is constant, meaning $\dot{Q} = \dot{Q}_0$ (see appendix 9.3). This may not be strictly true, as it is the fan drive that remains constant, and the beans change in density through the roast. Nevertheless, the assumption is safe because the fluid-bed coffee roaster contains a considerable amount of baffling that mitigates or causes only minor effects on the result.

[8] It should be noted that because air flow is not measured the bean load result is a qualitative. To make a quantitative measurement would require air volume flow rate, air pressure, and number of gas particles in the air (see appendix 9.3).

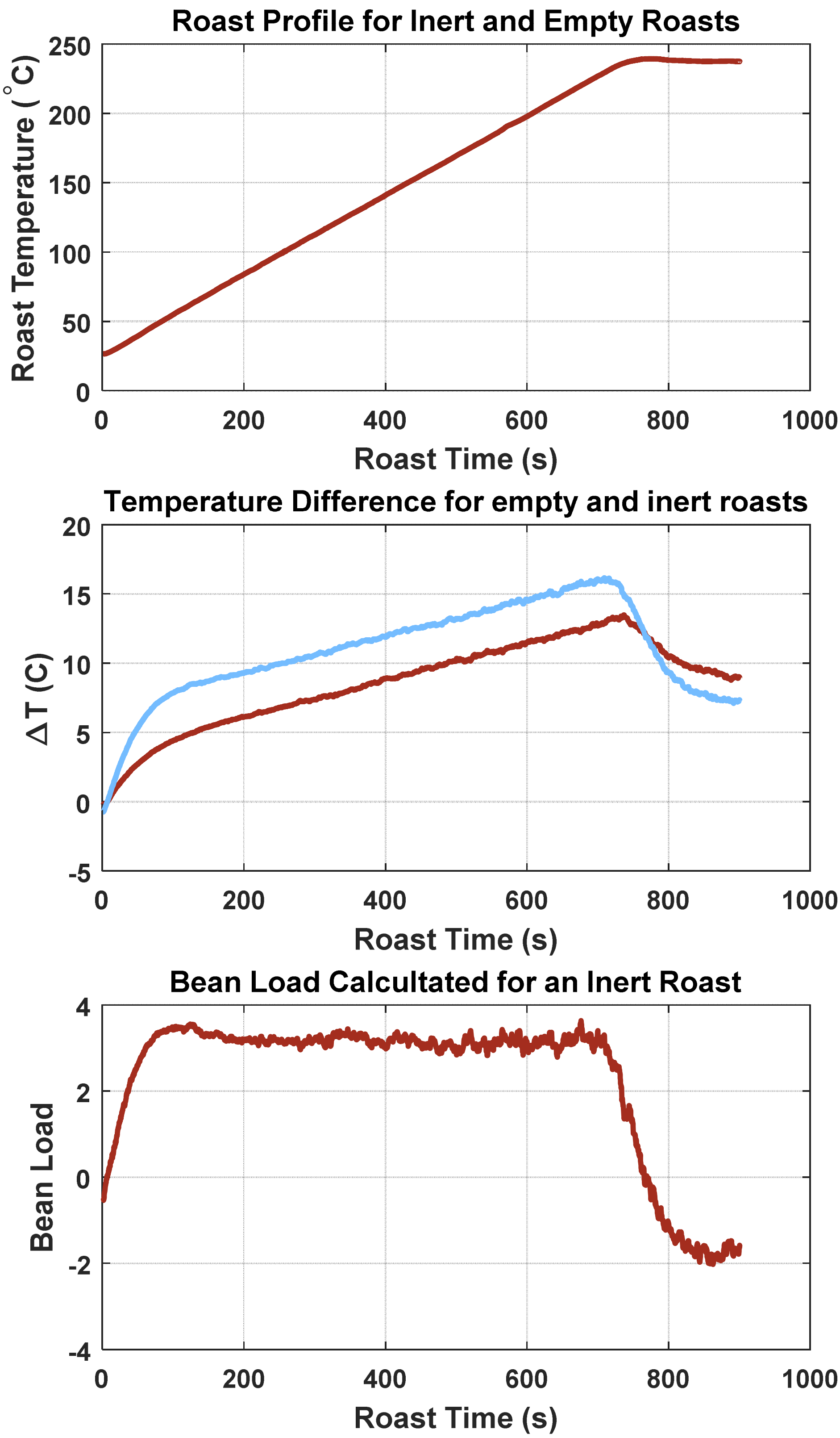


Figure 24. Showing the temperature ramp, the temperature, and the bean load of an empty roast.

4.4.3 Coffee Bean Load

When the bean load formula is applied to the data measured from roasting coffee, it shows how the coffee is thermally affecting the roaster system (Figure 25). The plot of temperature versus roast time in Figure 25 shows the temperature ramp, input, and exhaust temperatures from a large roast. These values produce the plot of the bean load (Figure 25b) filtered using the same median filter as in the case of the marbles. The bean load is seen to rapidly increase in the first 100 seconds in a manner similar to the marbles. This was attributed to the coffee and roaster's temperature stabilising after the start of the ramp. After the initial step, the bean load starts a near linear ramp until around 550s. Just after the 550 seconds there is a small upward bulge. Then at 600 seconds the trace levels out. First crack was recorded during the roast at 700 seconds and lasted 15-20 seconds. This aligns with a brief dip in bean load followed by a small peak. The temperature ramp reaches its maximum around 720 seconds (12 minutes). The bean load measurement after this point drops off rapidly. While the temperature is not increasing on the ramp it is not possible to be separate the transition from the background changes, making the bean load method unreliable after the change from ramp to constant temperature.

These characteristic aspects have been observed on multiple roasts. Only one data set is displayed here for reasons of clarity.

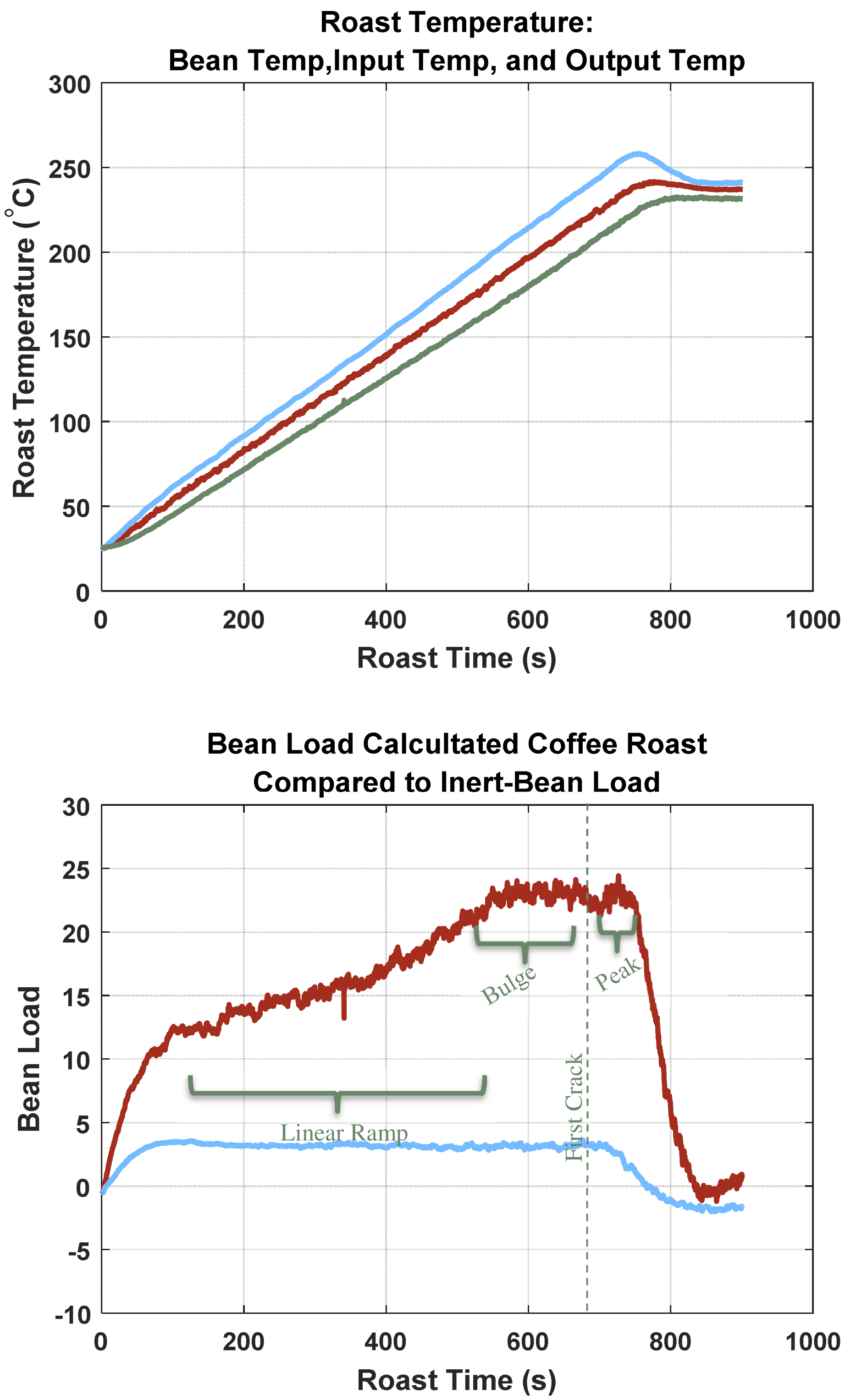


Figure 25. Temperature ramp and bean load calculated for a coffee roast (of the larger size). The top graph shows the input temperature (Blue), bean temperature (Red), and output temperature (Green). The bean load (bottom graph) of the coffee roast (Red) is compared to the bean load of an inert load (Blue).

4.4.4 Bean Load Analysis

What does it all mean? When the bean load is constant, no reactions are going on, the sample is neither absorbing extra energy nor producing any extra energy. This is seen in the inert bean case (Figure 24). Except for the initial settling phase and the post temperature ramp the inert bean load remains essentially constant, varying less than plus or minus a quarter of a unit.

In the case where the bean load is either increasing or decreasing, the sample bean is either absorbing energy or producing energy, respectively. Therefore, the increasing bean load ramp in the first section of the coffee roast is consistent with endothermic activity in the coffee. This is attributed, in the most part, to the heating and evaporation of water in the coffee that happens in the early part of the roast. It is also likely that reactions have started in the coffee that could also contribute to this. In other words, heat is being used to boil water and break down organic molecules. This is strong endothermic activity that appears to get increasingly endothermic over time. The bump just after 550 seconds implies that more energy is being used by the beans, so for that brief point the beans are more endothermic.

After the 550–second bump the trace suggests that the endothermic reactions are decreasing or they are being joined by exothermic ones. Exothermic reactions toward the end of roast are sometimes reported in popular literature. Net exothermic reactions under roast conditions were never observed in these experiments. Even though the reactions will eventually become exothermic if a roast is continued until the beans catch fire.

The next notably repeatable event is what appears to be a dip in the bean load around first crack. A dip in bean load at this point looks as if it could be a brief spurt of exothermic activity followed by a spurt of endothermic activity. However, it could also be an artefact created by the rapid change in bean density that occurs around first crack.

4.4.4.1 Fixed temperature bean load slew

In the end section of both the inert and the coffee bean roasts the temperature levels off. The bean load that accompanies this levelling off slews toward zero when this happens. The bean load calculation essentially measures thermal lag. This means, given a load measurement at a point in time, it shows the difference from the calibration load at the same point in time. Therefore, if there is no change in the input then the value will go to zero because the two points in time are indistinguishable from each other. In practice, what is seen is that it does not actually hit zero, this is attributed to the assumption made earlier that $F = F_0$. However, it is expected that the physical presence of a material in the chamber was changing the flow rate slightly. In other words, the zero calibration was not exact, but as the skew is so minor it does not create concern that this changes the meaning of the results.

4.5 Modelling the Thermal Behaviour of Batch Roasted Coffee

A behavioural model of the fluid bed coffee roaster and roasting coffee beans was created. This improved the understanding of the thermal processes acting on the coffee, as well as acted as a method of predicting the behaviour of roasting coffee. To achieve this, a method to simplify the system down into a one-dimensional (1-D) model was created.

4.5.1 1-D model of coffee roaster

The aim of this approach was to simplify the method of simulation by reducing the coffee roaster system down to a one-dimensional heat flow problem. To achieve this, the heat flow problem was considered as its analogous electrical circuit. This allowed the use of SPICE electronics modelling software to replicate the thermal processes in the coffee roasting chamber.

4.5.1.1 Initial empty chamber model

The initial step was to construct the equivalent thermal model of the empty roasting chamber. The first model produced, used a current source as a heat source and then represents the empty chamber as a combination of resistive and capacitive losses. The resistive loss represents heat lost out the sides of the roasting chamber. The capacitive loss represents the thermal capacity of the roasting chamber. The first part of Figure 26 shows an illustration of the coffee roaster and its electrical equivalence. The second part of Figure 26 shows an example of the equivalent circuit as it would be modelled in SPICE.

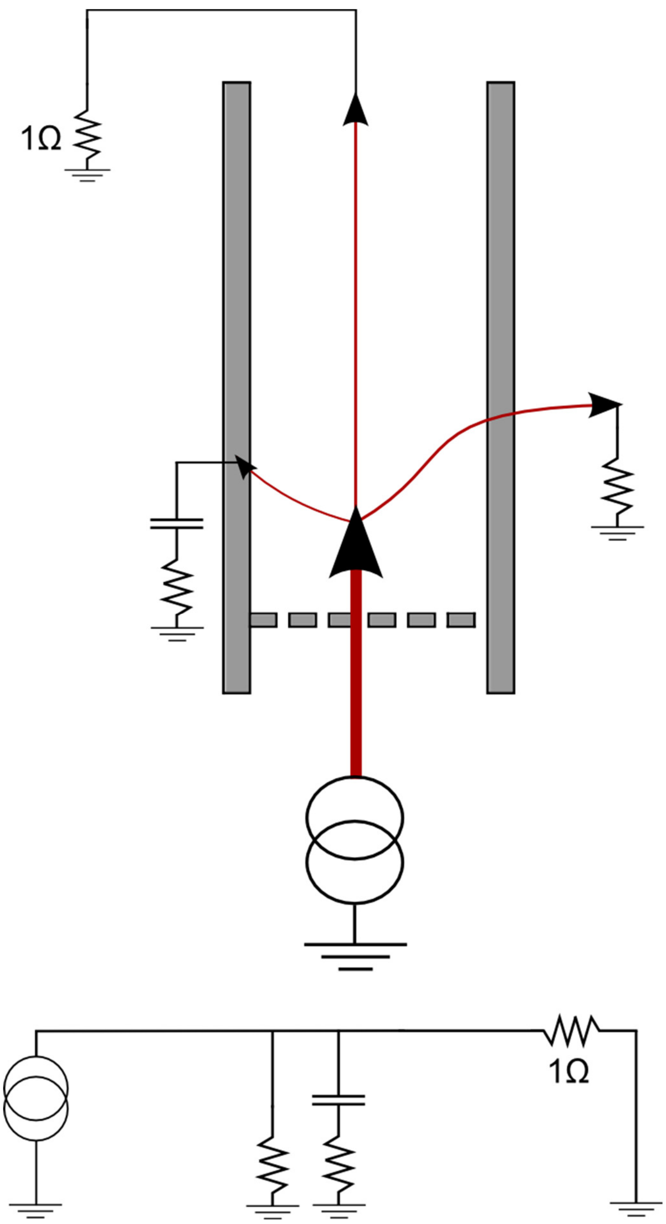


Figure 26. Basic single capacitor resistor coffee chamber model.

The modelled output was produced in SPICE using the input from an example blank roast. Values of various components were chosen to minimise the error between the model and experimental results. The SPICE model —with correctly chosen component values— produced the result in Figure 27. For the large part this model could match the experimental results. However, the model was noticeably lacking early in the roast and then after the temperature ramp had peaked. This model was shown to be lacking even further when applied to the inert marble case.

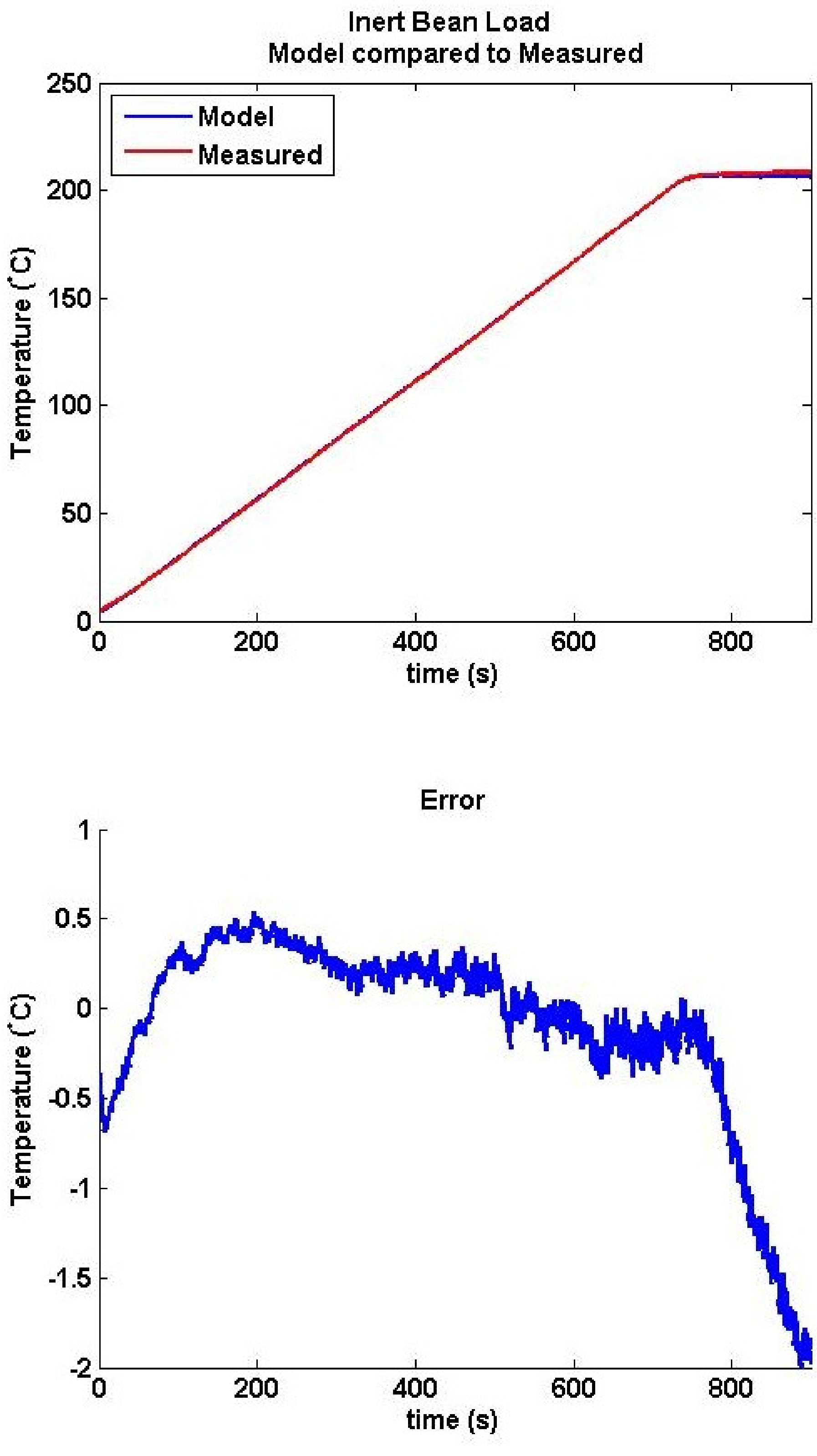


Figure 27. Modelled exhaust temperature using basic single capacitor resistor design (top); Error between model and experimental results (bottom).

4.5.1.2 Improvements to empty model

The first change made to the model was to the capacitance. Looking at other heat flow models showed that heat moves through a solid as an infinite sum of exponentials with ever decreasing time constants[55]. Therefore, the single resistor capacitor model was changed to a string of parallel resistor capacitors with decreasing time constants. This idea is represented in Figure 28. Although this method could have some improvement in the overall error it did not in any way solve the error spike that occurred after the ramp had ended.

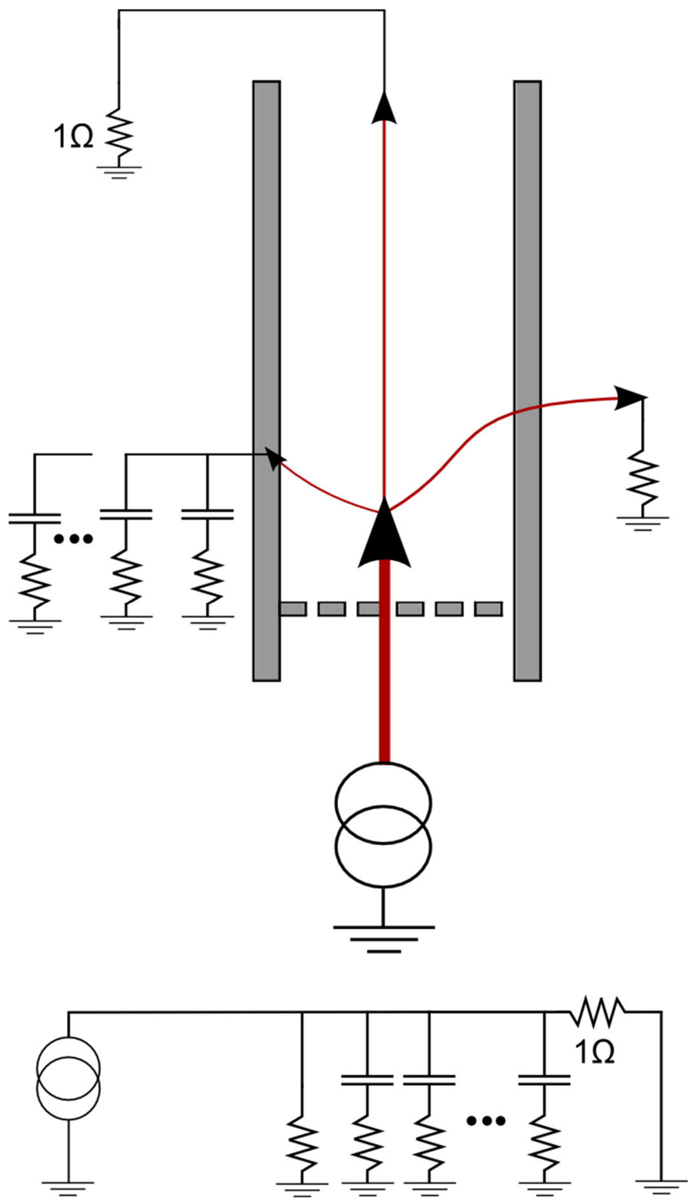


Figure 28. Layout of capactior model with split capacitor model.

4.5.1.3 Fixing the End of Ramp Error

The solution to fixing the steady-state error was to introduce a “pole” to the model. The problem with the initial model was it was matching the movement of the input temperature. The input notably overshoots the target temperature, as seen in Figure 25. This overshoot is not seen in the bean temperature (controlled input) or the output temperature.

The model was not representing the impedance to the heat flow created by the metal mesh that supports the coffee and the metal funnelling that directs air into the roasting chamber. To model this, the model of the roasting chamber was split in two and separated with a series resistor shown in Figure 29. The resistor behaves like a pole in a feedback loop, effectively adding a slight phase shift in the models output.

After tuning this new model produced the results in Figure 30. The resulting model greatly reduced the overall error. More importantly it also addressed the spike in error after the temperature ramp ended.

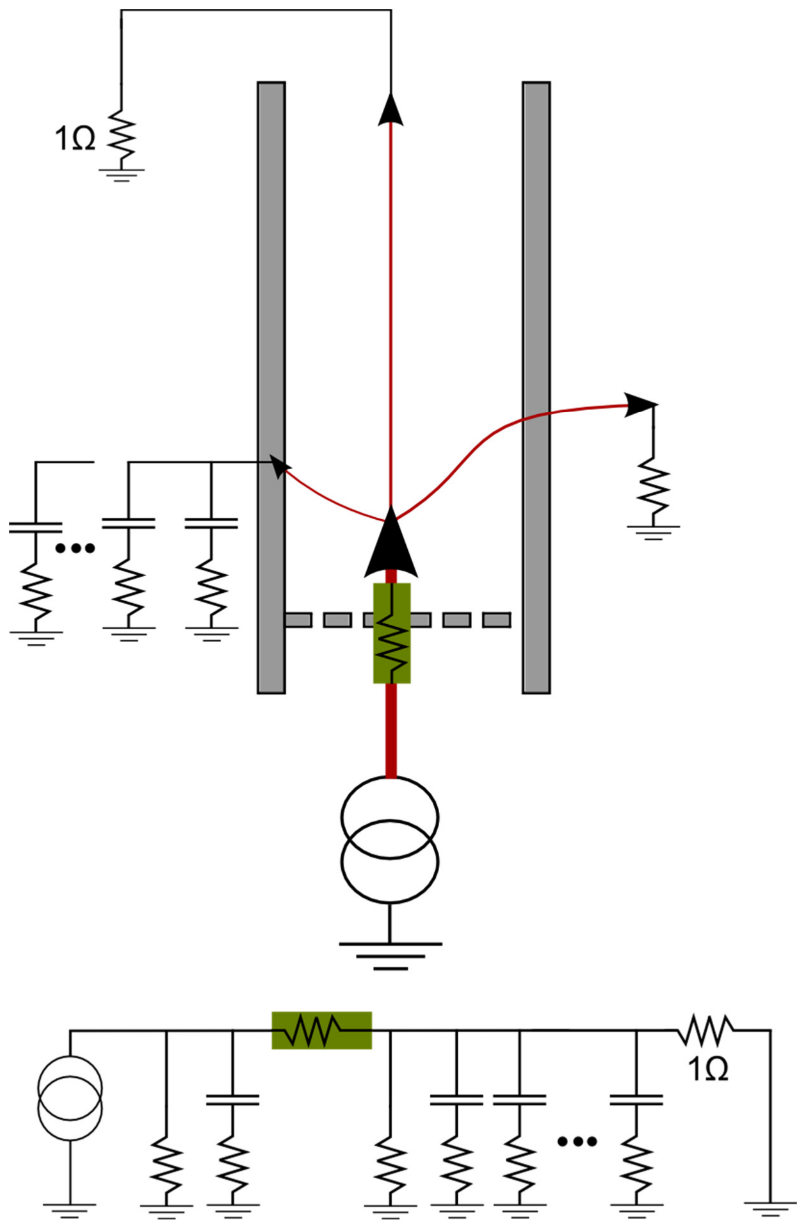


Figure 29. Circuit split by series resistor

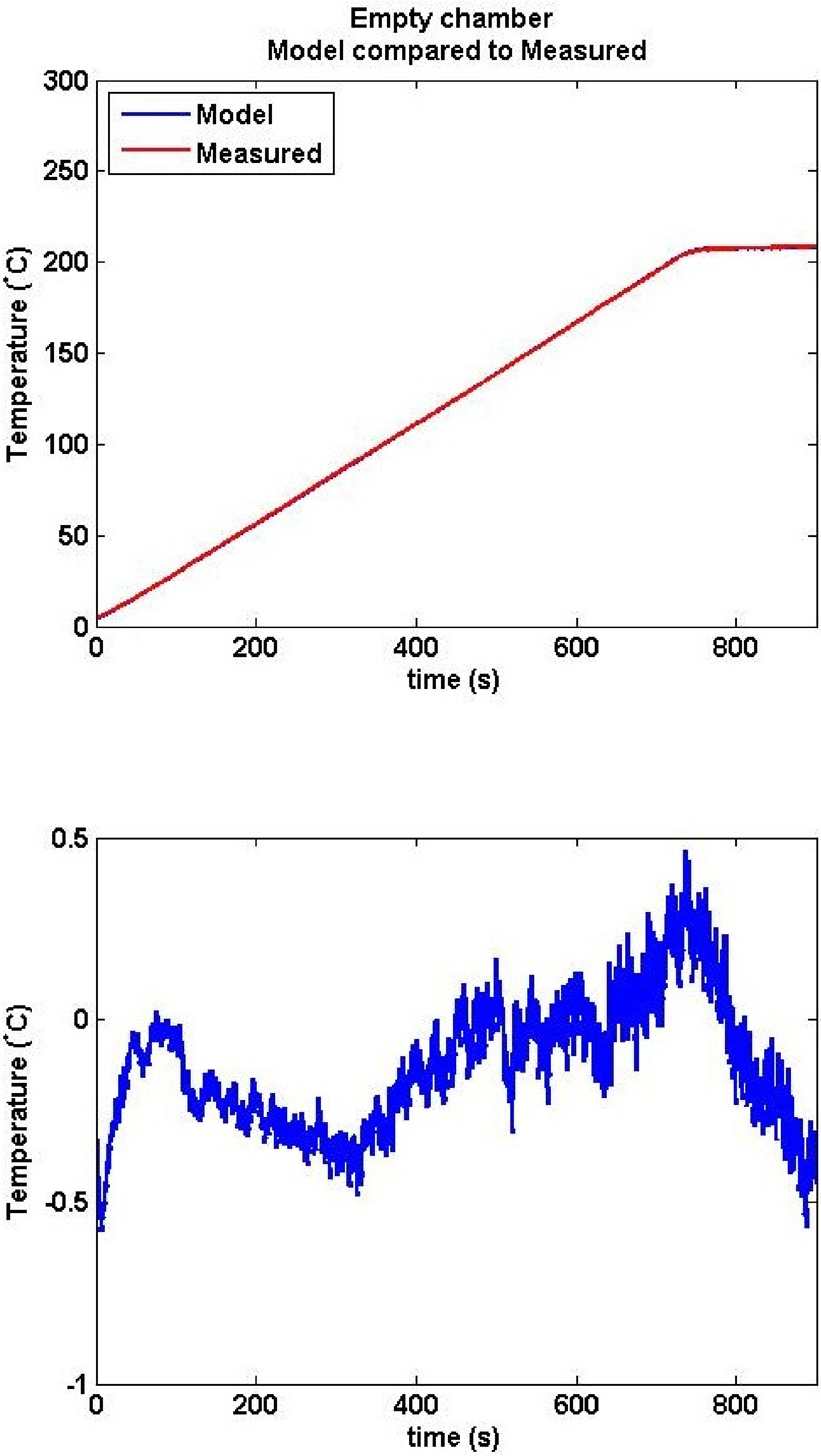


Figure 30. Result of adding a "pole" to the model. The overall error is reduced, as is the spike after the ramp ends.

4.5.1.4 Inert bean load model

The next step was to model an inert bean load. The model for the bean load was constructed in a similar manner to the chamber. The mass of inert beans can be modelled as a capacitive load. As the bean load is entirely inside the chamber it doesn't need a resistive component connected to ground as it cannot lose heat, except through the (already modelled) chamber. Additionally —as the beans impede the flow of air and heat— a series resistor was added introducing an extra pole. The circuit for this model is represented in Figure 31.The result (seen in Figure 32).

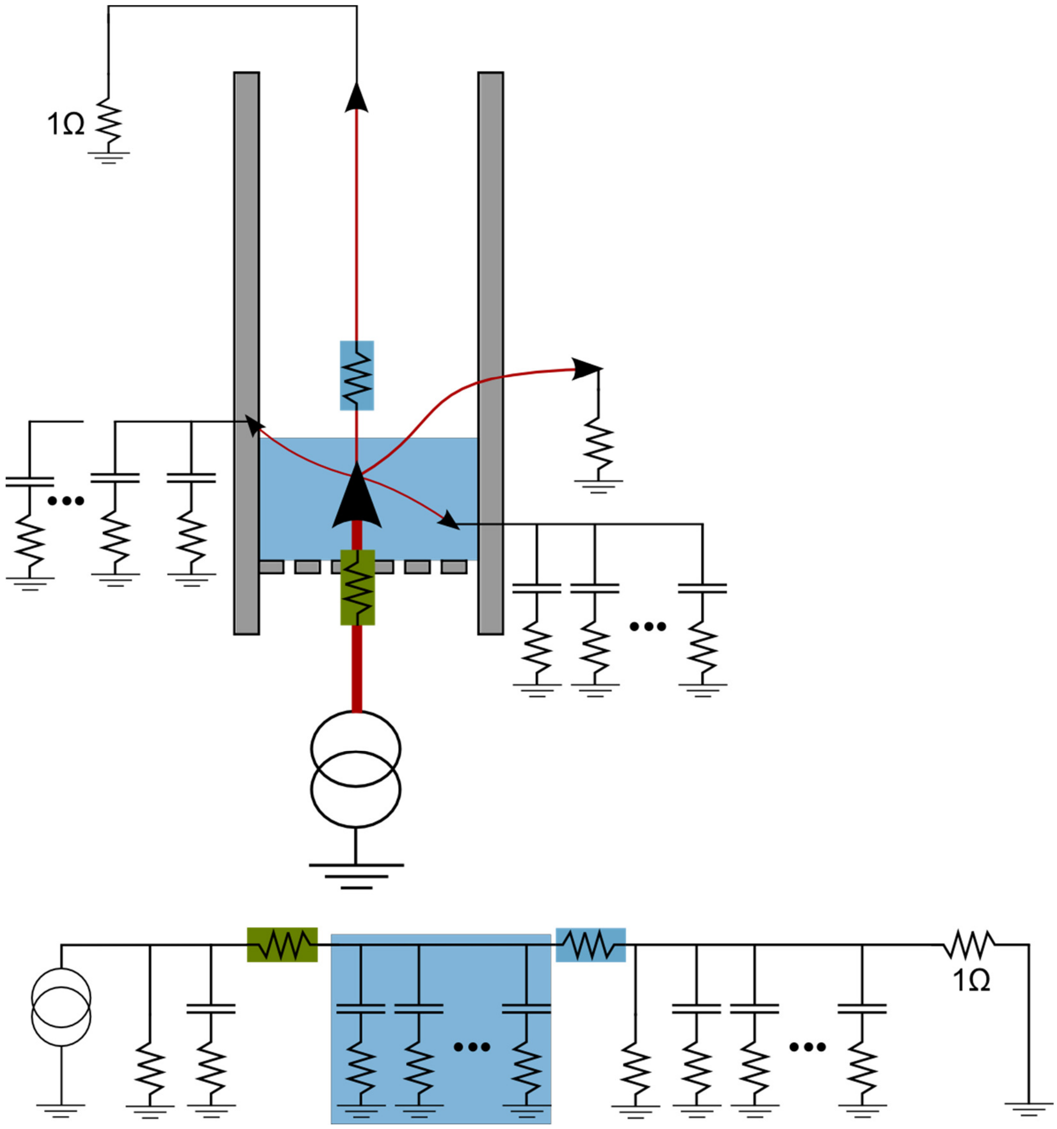
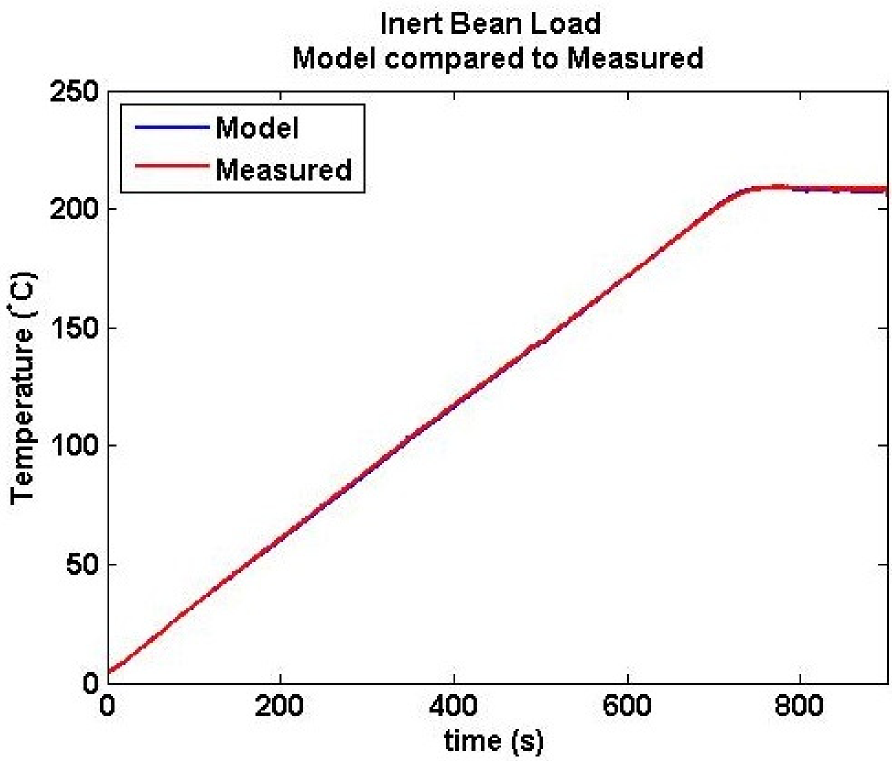


Figure 31. Inert bean load model. Bean load is added as a capacitive load a with series impedance.



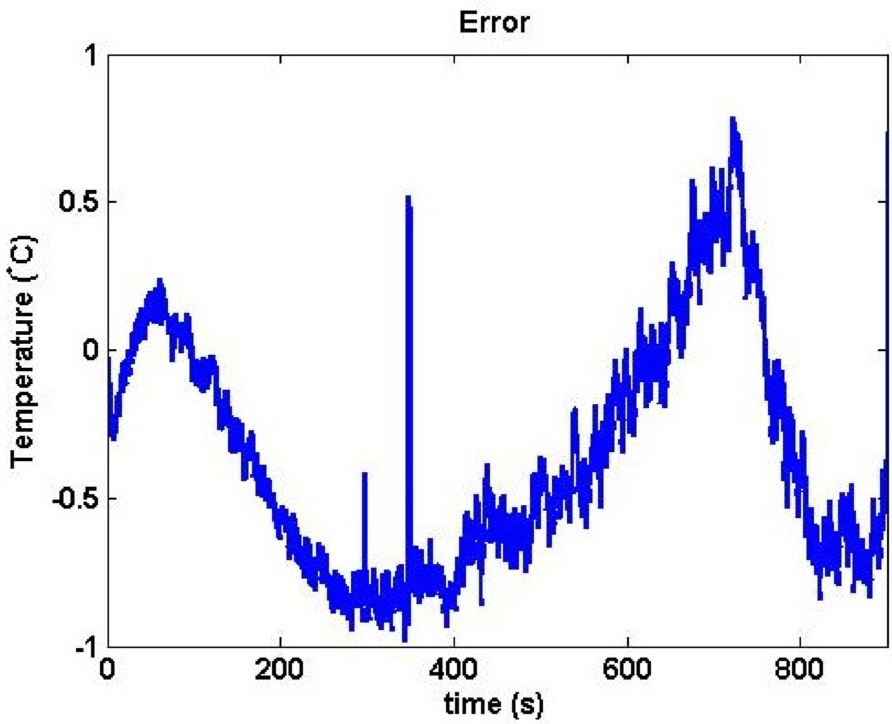


Figure 32. Inert bean load model results. Model compared to measured results (top). Error between model and measured (bottom).

4.5.1.5 Evaporation and Moisture Loss

The next step was to shift to an active coffee bean load model. The coffee bean load model requires a more complex design as it is changing during the roast. The assumption made, is that the measurable difference between the coffee bean load and an inert bean load can be attributed to the evaporation of the moisture in the coffee as the roast progresses.

The approach that was taken was to model the evaporation as a function varied current source that would draw charge out of the model. With current being analogous to heat flow, if the function was correct, it would represent heat lost from the system due to a changing factor. What was needed was a function or sub-circuit to represent the changing effect of moisture in the system.

The sub-circuit/function that achieved the desired result was a combination of a pre-charged capacitor and a function controlled current source. The voltage in the pre-charged capacitor represents the remaining moisture in the coffee. The current source draws charge out of the capacitor in a function related to the capacitor voltage and the model's current voltage. The function is represented by the equation:

$$I = K * |V(Bean) - 100| * V(Moisture)$$

Where *K* is a constant used for scaling. *V(bean)* is the temperature of the bean in the model. And *V(moisture)* is the voltage on the pre-charged capacitor. This current source is duplicated and used to draw charge from the bean model. Additionally, the current source is restricted to only work when the temperature is over the boiling point of water. Therefore, current is drawn from the circuit in proportion to the remaining moisture and the systems temperature over 100 degrees. This is represented in the diagrams in Figure 33. The full SPICE netlist for this circuit can be found in the appendix.

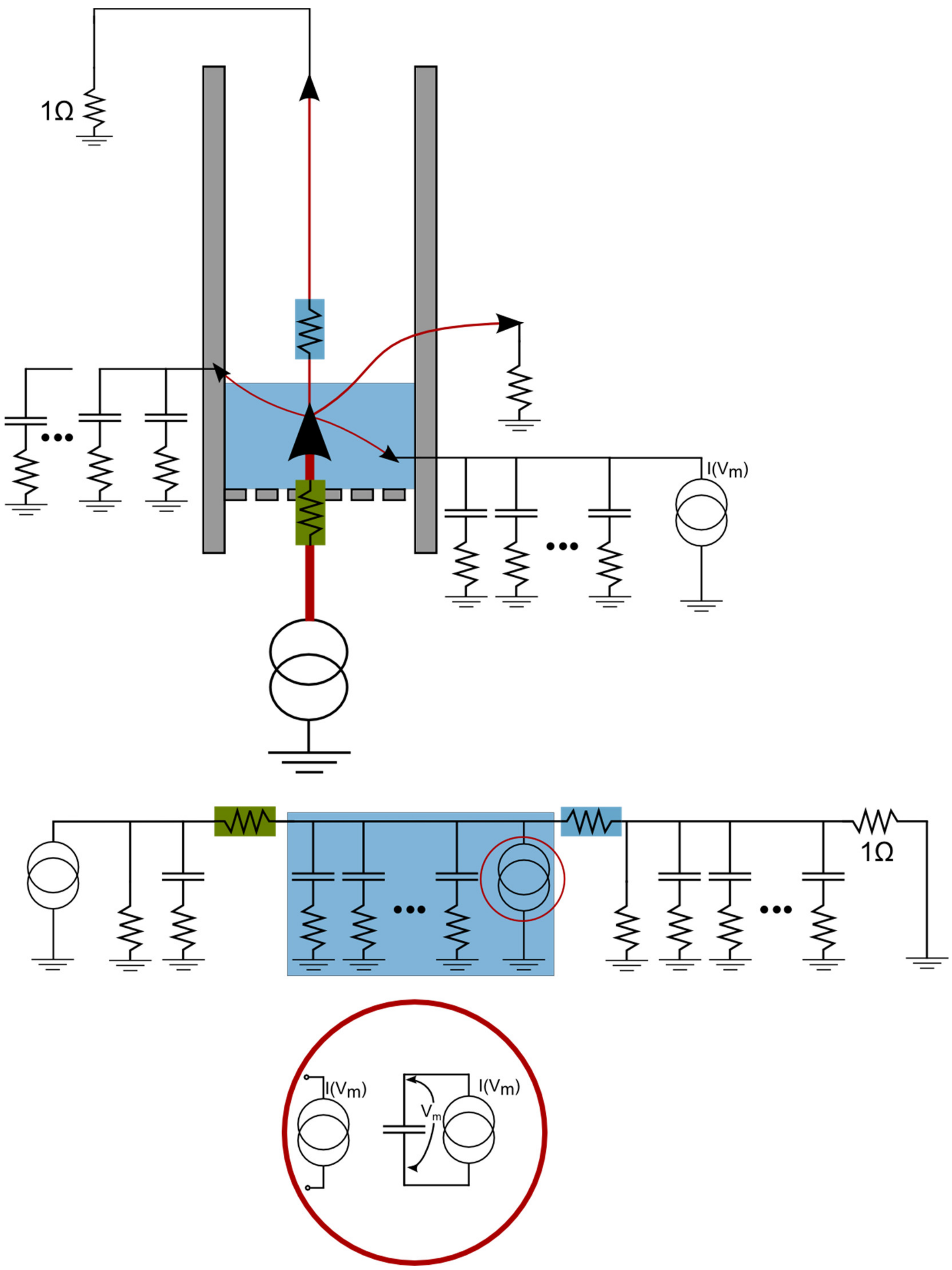


Figure 33. Model of roasting chamber, bean load, and evaporation. Evaporation is modelled as a current source whose current is a function of the voltage on a capacitor.

4.5.2 Evaporation Model Results and Comparison to Measured Data

It should be noted that as the model becomes more complex it adds additional variables that need to be tuned. This makes tuning more difficult and artefacts of poor tuning are harder to remove from the final model. The results from the evaporation model are displayed in Figure 34. Once tuned, the coffee model with evaporation fits the measured results remarkably well. On closer examination, it appears that evaporation accounts for most of the thermal action that occurs in the real coffee when compared to inert coffee.

There is a noticeable error in the model at around 400 seconds. This error can be attributed to tuning. It is created when the model starts to apply evaporation. The only error in the model that cannot be accounted for as an error in tuning is the blip during and after first crack.

The blip, around 750 seconds, is not accounted for in the model. Which implies that it is not directly caused by the energy lost to heating the bean or evaporating moisture. The previous assumption was that the oddity was a dip in the bean load making it appear more exothermic. However, after modelling bean load, what is observed is that the bean load starts to become more exothermic as the moisture runs out. This means that the oddity is not the dip but the subsequent spike.

A spike in bean load represents an endothermic process taking place. During first crack the beans are rapidly expanding and releasing gas. As first crack is underway at this point a more endothermic load makes sense, because the rapid expansion of evaporating gas is an endothermic process.

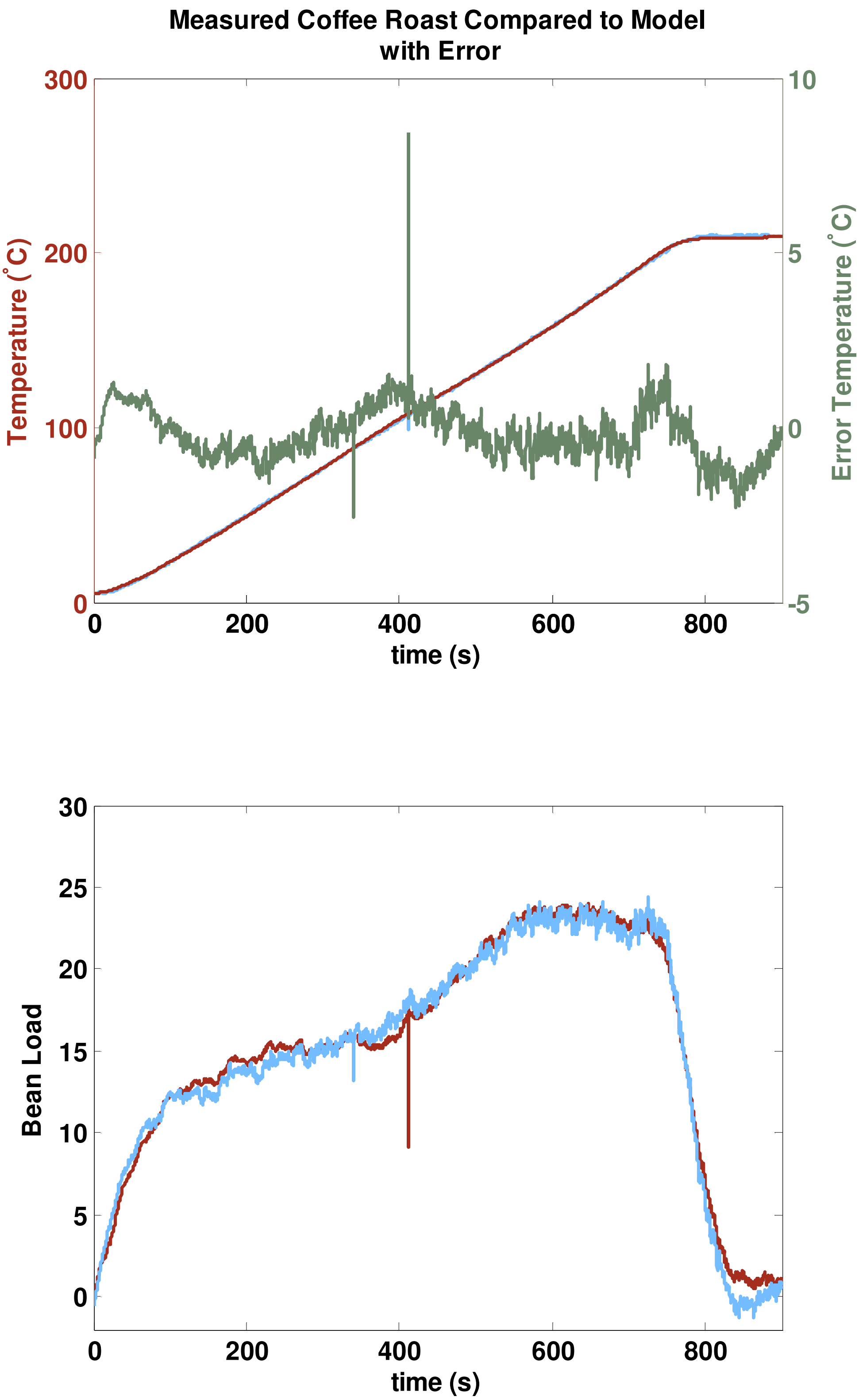


Figure 34. Results from bean load with evaporation compared to measured results from the larger coffee roast (top) Red – Model output, Blue – Measured results, Green – Error. Bean load calculated using the thermal model and the measured results (bottom).

4.5.3 Reanalysing Bean Load with the Reference Model

The construction of the model allows for a reanalysis of the behaviour of the coffee's bean load. For the most part, the model helped solidify the previous stipulations about the behaviour in the beans. The model did help with understanding the odd transient at first crack. By considering the model, the thermal action in the bean can be broken down into sections of interest. Initial heating, evaporation, first crack, and end of ramp slew.

During the initial stages of the roast, energy is lost in heating the coffee. At this stage, the coffee behaves, thermally, like an inert load. Any chemical reactions occurring during this heating period are too small to have any measurable effect on the results. During this section, the model is essentially just charging capacitors. The model brings this section to an end when the beans reach the boiling point of water.

After the beans hit the boiling point of water the, thermally, most visible reaction starts, evaporation. At this point, the model starts drawing charge out of the system at an ever-decreasing rate. This behaviour matches the heat lost to evaporation in the real coffee data. As the moisture (in the coffee) and charge (on the model capacitor) deplete, the rate of heat/charge loss decreases. This occurs until the loss due to evaporation becomes so minimal that bean load starts to drop. It is at this point that the model and coffee start to disagree.

As first crack starts, the coffee's bean load temporarily increases and moves away from the model's whose predicted load is decreasing. Previously the dip appeared to be the coffee acting more exothermically[9]. However, the model shows that the expected bean load starts to fall even before first crack, or the ramp levelling out. The increase that comes with first crack means that the system is acting more endothermically during this period. This is likely due to the rapid expansion of gasses and volatiles being released from the coffee having a net endothermic effect.

[9] This assumption was made because in the lower mass test, where this blip is not visible above the noise, the bean load remains flat.

4.6 Conclusions

This chapter discusses the design and construction a fluid-bed coffee roaster. It also discusses the use of temperature as a method of controlling a coffee roast, and potentially detecting the degree of roast. It looked at the idea of using control output to track changes in the coffee roast. There was no detectable relationship between the control input and the roasting coffee. After this it looked at the temperature difference between the roasting chamber's temperature and its output temperature. From this data, the idea of bean load was conceived.

Bean load represents the thermal load that adding coffee beans to the chamber creates. It is calculated as the difference between a loaded chamber and an empty chamber's ΔT — where ΔT is the difference in chamber input and output temperatures. This theory was tested with an inert load of glass marbles. The glass marbles produced a level bean load as would be expected.

When the bean load calculations were applied to the temperature data from a coffee roast it produced a graph that reflected the changes coffee experiences during roasting. The bean load shows the expected endothermic period in the early section of the roast that is largely dominated by the evaporation of water. The endothermic reactions are shown to lessen in the middle of the roast. There was also shown to be a repeatable dip in bean load that occurred during first crack.

To gain a better understanding of the coffee's thermal roast behaviour a SPICE model was designed to model the coffee's thermal characteristics. The model worked on the analogous behaviour between heat flow and electrical current. The model accounted for heat lost to the coffee's thermal mass and to evaporation. The only noticeable transient that the model did not account for was the spike in bean load after first crack.

4.6.1 Detecting Second Crack

The coffee roaster was not able to maintain the increasing ramp — required for useful bean load calculations — until the coffee reached second crack. Therefore, it cannot definitively be said that there is a repeatable transient in the bean load caused by second crack. Additionally, there is no notable variation between the model and coffee bean loads after the ramp ends that would signify that second crack had occurred.

Second crack itself may cause a spike like the one created by first crack. However, the first crack bean load spike is not visible until first crack is well under way. If second crack were to produce a spike in an analogous manner it would not be detectable early enough to be able stop the roast at a point considered before second crack.

4.6.2 Final Thoughts and Improvements

The measurements taken were sufficient to test the limits of the coffee roaster and make judgements on the merits of the bean load as a control scheme. It would be possible in future work to make improvements to the coffee roaster to improve the quality of these measurements. As this method of measurement did not provide the desired result and therefore it was decided to not continue with this line of investigation.

Although this approach did not give the desired result of detecting second crack it did produce a somewhat macroscopic look at the thermal behaviour of coffee during roasting. This method and approach could be taken further to better examine the calometric nature of batch roasted coffee. This would require sizeable changes and redesign of the coffee roaster.

1. A larger heat source in the coffee roaster. This would allow for the roaster to reach second crack with a ramp temperature profile. Therefore, second crack's effect on bean load could be tested during a temperature ramp.
2. The addition of flow sensors. This would allow a more thorough investigation of how changing the air flow affects bean load. Additionally, it would allow the bean load to be calculated even when the input fan speed is modified to control roast temperature.
3. Improve the signal to noise ratio of the bean load result. Making changes to the coffee roaster such as; allowing for a larger sample of coffee beans; using multiple points of temperature measurement on input and exhaust; improving the overall insulation. These types of changes would mean a stronger (and hopefully less noisy) signal from the bean load. This would

mean finer changes in the coffee beans' chemistry could be reflected in the bean load.

The main conclusions from this experiment are:

1. Straight bean temperature measurement did not return interesting information about the state of the coffee in the roast.
2. A straightforward model of coffee's thermal properties could predict most of the coffee's macro thermal behaviour (except for first cracks endothermic blip).
3. A macroscopic look at coffee's thermal behaviour was possible during batch roasting using basic temperature measurement and coffee roasting equipment.
4. The bean load produced an interesting measurement of coffee but it was ultimately not able to do the job of detecting second crack. [42]–[48]

5 Online Microwave Moisture Measurement of Roasting Coffee

5.1 Chapter Introduction and Summary

The goal of this chapter is to measure the loss of moisture in the coffee as it roasts. Microwave radiation can be used to measure dielectric properties of substances; in this case microwave measurements are used on coffee during roasting. This allowed for the observation of the coffees' changing dielectric properties during roasting. The thought being that the dielectric properties will change as moisture in the coffee evaporates during roasting. The plan was to use these measurements to make an online measurement of the coffees' moisture content. The moisture present in beans was measured during the coffee roast with the expectation of achieving an appropriate roasting duration and the correct end-point.

To make this measurement a coffee roasting chamber was designed and built that was intended to be connected to a network analyser. The chamber built to achieve this was a stainless-steel roasting chamber that fitted in the place of the glass roasting chamber on the coffee roaster. Using the network analyser measurements were then taken on the coffee's changing dielectric.

The measurements taken of coffee on in a fluid-bed were found to be very noisy as a side-effect of the movement of the beans. A method was designed to clean up and make sense of the measurements. Then the results were compared with other measurements to make sense of them and understand them in the context of coffee roasting.

The measurements showed what was expected from changing temperature and moisture loss in the coffee during roast. The measurements did not show a "smoking gun" or definitive waypoint that could be used in the detection of second crack. Even though it didn't show the desired transient, it was an interesting result showing a repeatable progression that could be used as part of a larger solution or independently in a similarly noisy environment.

5.2 Microwave Measurement of Moisture

The microwave measurement of moisture of grains has existed in various methods since the eighties [63]. The concept this method of moisture measurement is based on is that the dielectric properties of the water in grain have a greater effect on electric fields than the rest of the material in the grain.

Microwave moisture measurement techniques fall into four categories [64], [65] (Figure 35): the 1-port open-ended method [66]–[68], the 2-port transmission method [69]–[75], and 1- or 2-port resonant methods[76]–[81]. All utilise the dielectric properties of water. The 1-port approach typically measures the change in the electrical fields at the end of a probe via a measurement of S11[10]. For example, Filali et al. [66] extracted moisture content in concrete from the S11 of an open-ended coaxial probe pressed against the sample. Lawrence et al. [74] used a 2-port transmission method to measure the moisture content of grains that take the place of the dielectric support in a coaxial structure. Resonant techniques use the cavity perturbation method to find the permittivity of a sample. By measuring the change in the resonant frequency and Q of a cavity when empty and when the sample is present the sample dielectric properties may be determined [65], [78], [82]. The resonant methods rely upon some assumptions. The electric fields in the cavity must be negligibly changed by the sample, and that the electric fields typically need to be uniform over the volume of the sample.

[10] S11, also known as the reflection coefficient, is a measure of the amount of energy reflected from a system as a given frequency.

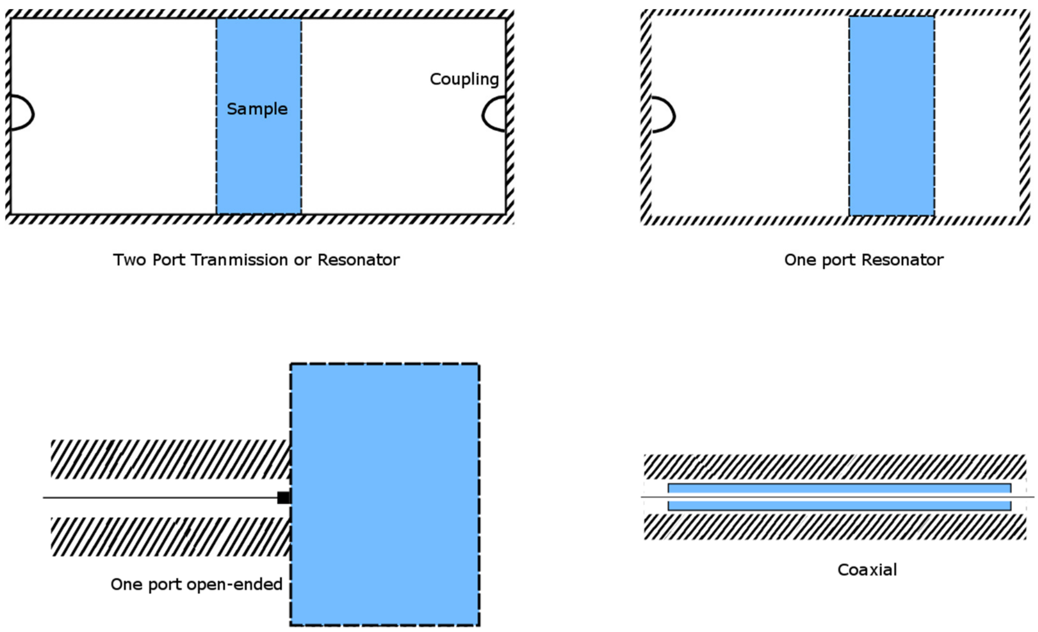


Figure 35. The different methods of making moisture measurements using electric fields.

5.3 Microwave Rig Setup

5.3.1 Roasting Chamber Design

The choice of measurement method was limited because it needed to take moisture measurements while simultaneously roasting coffee. The roasting chamber was designed so that it could facilitate both functions shown in Figure 36. It used the 1-port resonator method. This measurement method was chosen because of the physical constraints of the system. The roast chamber was constructed out of stainless steel pipe machined with threads at each end. The threaded sections were used to attach perforated stainless-steel disks. Hot air for roasting was pumped through a perforated disk at the bottom and flowed out another perforated disk at the top. The microwave energy was admitted in the side of the wall connected to a coupling structure. The structure was made from a male N-type connector mounted to the side of the chamber. The connector was shorted to the chamber using a loop of wire. A CAD outline of the chamber is included in the appendices.

This resonator design worked as a coffee roaster; however it was not ideal for making moisture measurements. This was because it failed to meet the two assumptions that resonant methods rely on[11]. For this reason, the measurement of

[11] 1) The sample is in a uniform electric field. 2) The sample does not significantly change the shape of the electric fields.

the absolute moisture of permittivity of the coffee was not targeted. Instead a qualitative measure was devised to identify the loss of moisture in the coffee by watching the change in frequency and impedance of a resonant peak during the roast.

Figure 36. Stainless steel roasting chamber used as the 1-port microwave resonator

The basis for this idea can be seen in how cavity resonance is calculated. The formulas for calculating the frequency of resonant modes (both transverse magnetic and transverse electric) in a cylindrical resonator are below.

Transverse Magnetic mode: $f_{mnp} = \frac{c}{2\pi\sqrt{\mu_r \varepsilon_r}}\sqrt{\left(\frac{X_{mn}}{R}\right)^2 + \left(\frac{p\pi}{L}\right)^2}$

Transverse Electric mode: $f_{mnp} = \frac{c}{2\pi\sqrt{\mu_r \varepsilon_r}}\sqrt{\left(\frac{X'_{mn}}{R}\right)^2 + \left(\frac{p\pi}{L}\right)^2}$

Where c is the speed of light, μ_r is the relative permeability, ε_r is the relative permittivity, R is the radius of the cylinder, L is the length of the cylinder, X_{mn} is the m-by-nth root of the Bessel function, X'_{mn} is the m-by-nth root of the derivative of the Bessel function, and m, n, p are the mode numbers for any given mode. The equation for resonant frequency is made up of two parts, the shape of the cavity, and the speed of light in the cavity. If the shape of the cavity and the permeability is fixed but there is a change in the permittivity, that will result in a change in the resonant frequency of the cavity. That is the goal of this experiment. The math here assumes that the permittivity of the cavity is uniform. However, in the roasting experiments, the coffee will introduce an increased permittivity densely packed in the lower section of the chamber. This makes it hard to predict what behaviour the chamber will exhibit during roast. The solution was to make measurements of the chamber and observe the changes with and without coffee.

As a side note, the solutions to the lowest possible frequency modes, both TM and TE, in the stainless-steel coffee roasting chamber are as follows: Transverse Electric: $f_{111} = 2.88\,GHz\,(3\,s.f.)$; and Transverse Magnetic: $f_{010} = 3.69\,GHz\,(3\,s.f.)$.

5.3.2 System Setup and Changes

The base roaster and its control remained mostly unchanged for these experiments. The major difference between this set of experiments and the last was the removal of the “in bean” thermocouple. This was removed so that it would not interfere with microwave measurements taken inside the resonator.

The chamber was connected to the coffee roaster and the system was connected as in Figure 37. Measurements were made by a network analyser. The network analyser was in turn linked back to the controlling computer via a GPIB interface. During roasting, the control computer performed 201-point complex S11 sweeps every 0.25 seconds. Longer sweeps improved resolution but slowed sample rate so were used only for non-roast tests.

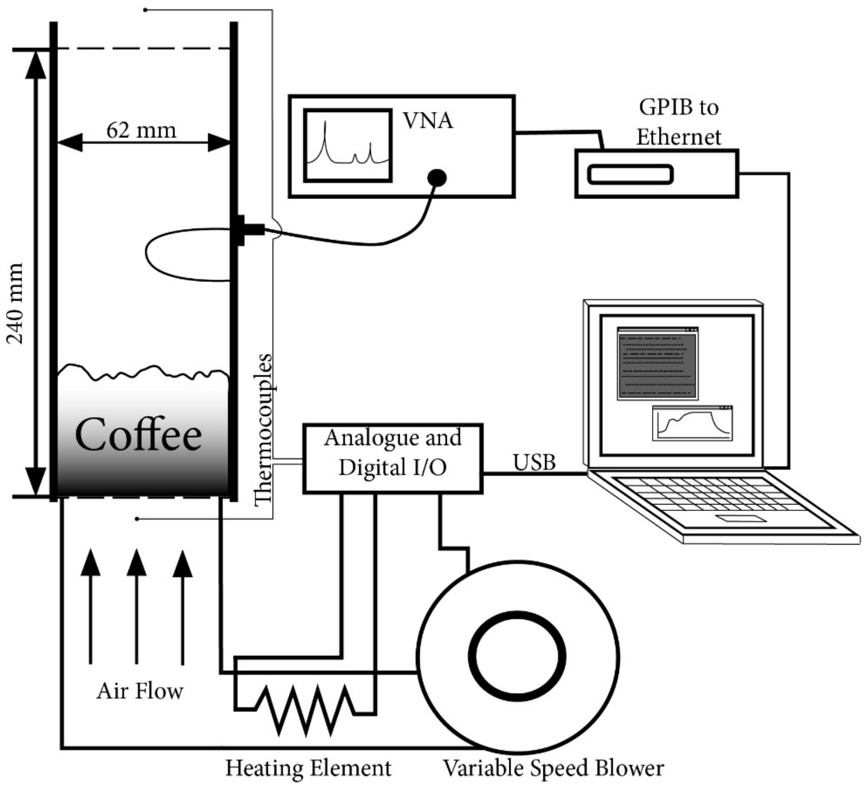


Figure 37. Functional layout of the coffee roaster and network analyser setup. It was setup like the original, with the exception that the thermocouple measuring the temperature inside the coffee has been removed. The stainless-steel roasting chamber was coupled to a network analyser. A computer logged data from both the network analyser and the thermocouples as well as controlling the roast temperature.

5.4 Initial Coffee Roast Measurements

The roast chamber design limited the options for taking measurements. The goal was to identify resonant peaks and track how they move during roasting. Then by observing the movement draw conclusions on how the coffee was changing by the changing fields. The first graph in Figure 38 shows a set of S11 magnitude measurements taken from a coffee roast with a step profile. The measurements show change as the roast progresses. However, from this data it is hard to see any discernible pattern as the roast progresses. On top of this, while the coffee roasting was in progress, successive measurements were very noisy. This created several issues that needed to be addressed before the method’s ability to make any roast predictions could be evaluated.

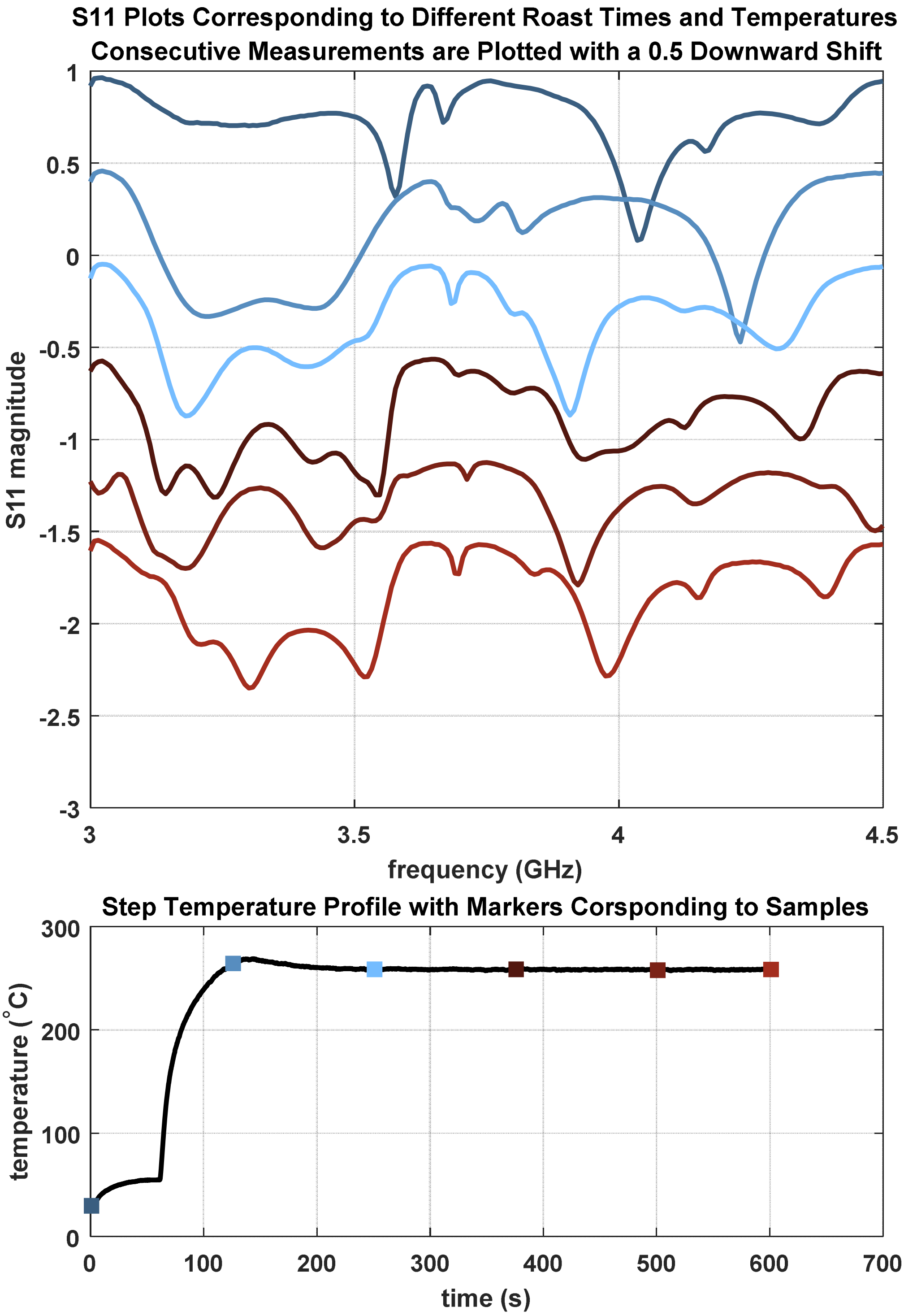


Figure 38. S11 measurement plots taken of coffee at various times during a coffee roast. An offset has been added to consecutive measurements so that they can be viewed separately.

The first problem that needed to be solved was finding a reliable peak to track over the course of the roast. The magnitude of S11 was not initially useful because of the peaks not having any easily discernible patterns. After considering the data further, it was found that the real component of the impedance (Z-real) had a peak with a discernible pattern as the roast progressed.

The peak — seen in Figure 39 — shifted between 3.2 and 3.5 GHz over the course of the roast. This peak can be seen to diminish and decrease in frequency over the course of the roast. In the later stages of the roast it started to increase in frequency and amplitude again.

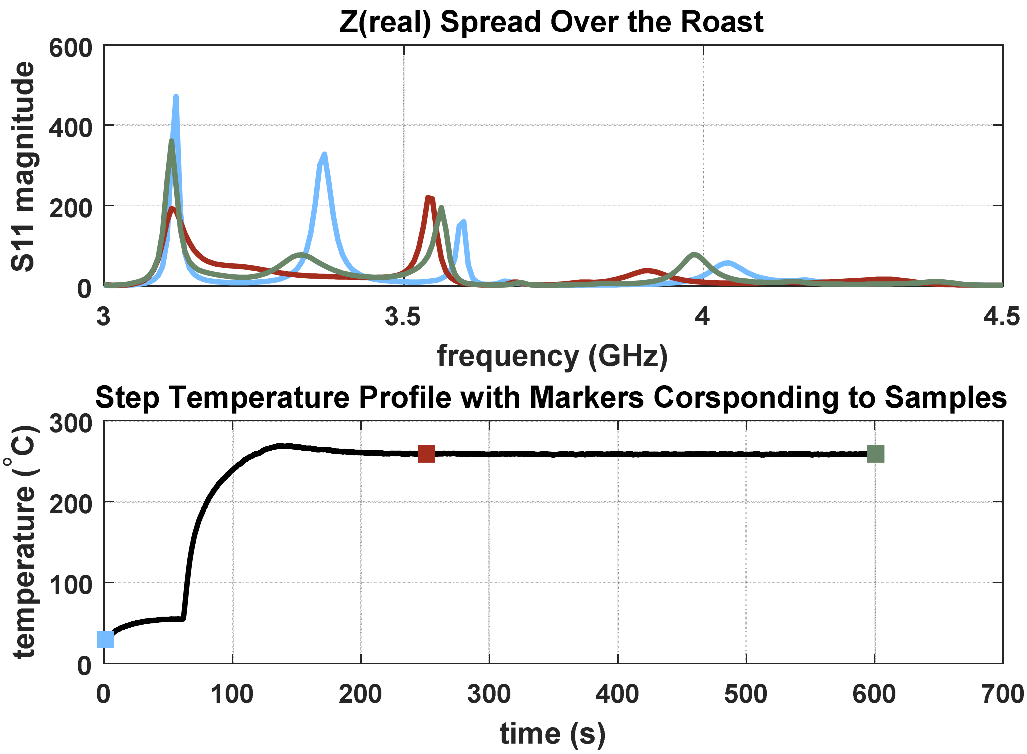


Figure 39. Real impedance calculated from S11 at various points in a roast.

Once a peak was identified whose changes could be tracked through the roast what needed to be identified was which factors affected it during the roast. The problem was that roasting is a messy process with a lot going on. Not only was the coffee losing moisture, it was also, moving, being heated, and changing in size. The expectation is to see a noisy signal that behaved erratically.

5.5 Making Sense of the Data, the First Two Major Factors

The major factors observed that affected the resonant peak measurement are, the moisture content[12], the sample temperature, and the movement of the coffee sample. Tests run on the different factors allowed for an understanding and connection between the physical changes and the measured results.

5.5.1 Test on Varying Moisture Content

The first measurement test was on moisture content. This was done using a simple experiment that varied moisture levels and measured effect on the resonant peaks.

It is difficult to ascertain what effect the moisture in the coffee will have by looking at literature on the dialectic properties of water. Martin Chaplin's website on "Water Structure and Science" gives a good 1800 word summary on the interaction between water and microwaves[83]. In this summary Chaplin includes some graphs based off the models created in T. Meissner et al's work looking at the complex dielectric constant of pure and sea water[84]. The model expresses the relationship between water's temperature, electromagnetic wave frequency, and complex permittivity. The model shows that for pure water, and frequencies below 10 GHz, both real and complex dielectric components decrease with increasing temperature. However, this only holds true for pure water.

What is noticeable about T. Meissner's work is that it looks at both pure water and sea water. In the case of water with salt in it the dielectric loss (complex component of dielectric) flips and increases with temperature increase. The paper also shows that increasing salt concentrations increases this effect. The assumption is that the moisture trapped in the coffee is more likely to behave like the non-pure water and have an increased permittivity. However as mentioned the exact effect of the moisture is easier to test than predict from literature.

The experiment worked by suspending different masses of tap (non-pure) water in a sponge. The sponge was sized and placed in the roasting chamber so that it

[12]An assumption was made that the moisture content's absolute permittivity is a significant proportion of the overall permittivity [64]. This means that the change in moisture will represent a large proportion of the overall change in the measurement.

occupied space and volume like that of the coffees' during roast. Measurements were taken at room temperature. The sponge was chosen because it had an insignificant effect on the system.

The graph in Figure 40 shows the result of the sponge moisture experiment. The resonant peak of interest shows significant change as the moisture content changes. As the moisture content increases the peak both decreases in frequency and amplitude.

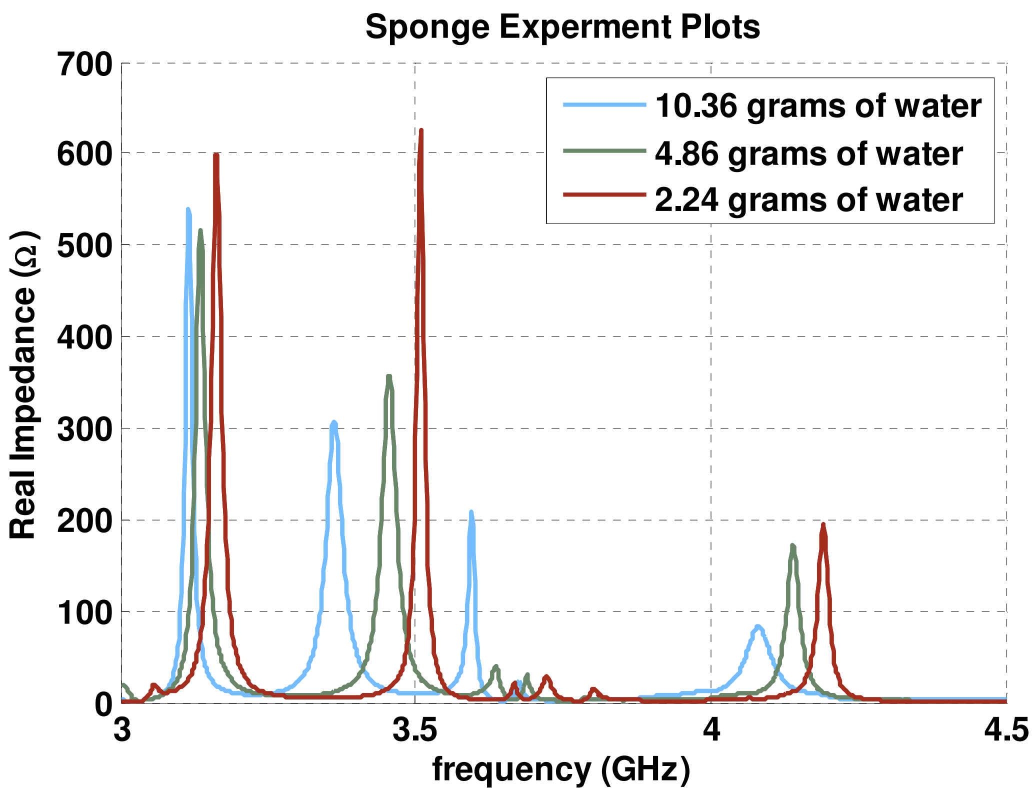


Figure 40. Z-real plots produced by suspending different masses of water in sponge.

When comparing a mass of water suspended in a sponge to the moisture in coffee, the moisture in the coffee of the same mass was observed to have only a slightly greater attenuating effect. This is shown in Figure 41 which compares green coffee with 11.5% moisture (8.05 g) with the same mass of water suspended in a sponge. This supports the assumption that the non-moisture component of coffee has a much smaller effect on this form of measurement.

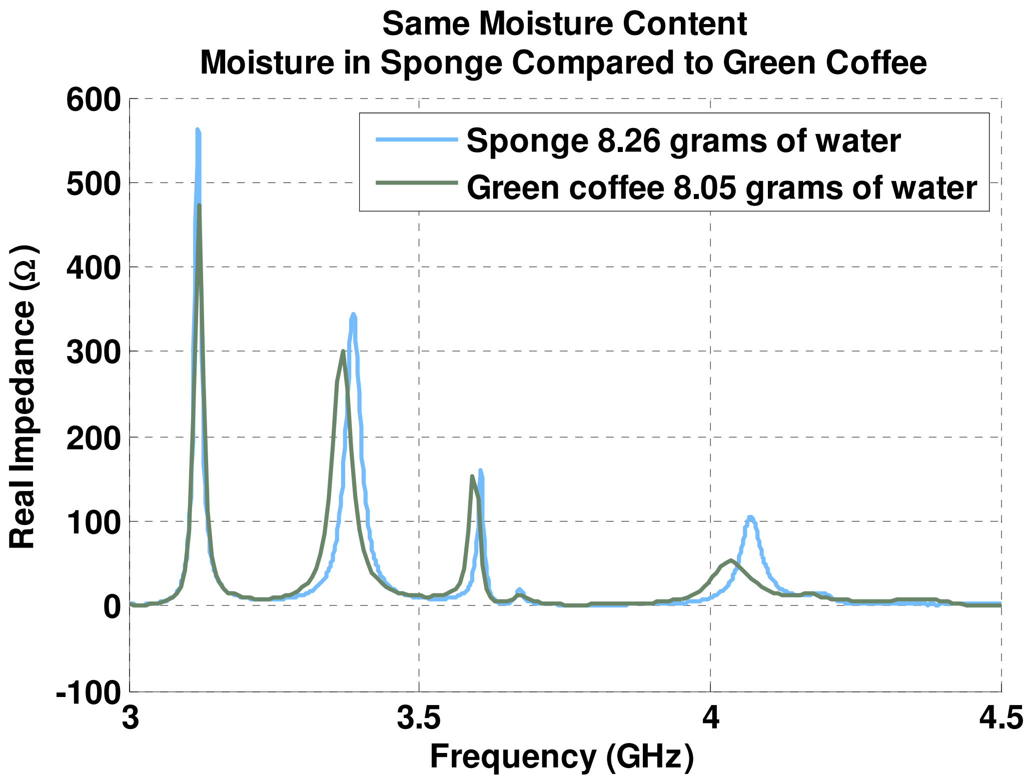


Figure 41. Comparisons of similar masses of water in different mediums.

5.5.2 Observing the Effect of Changing Temperature

The other major factor that affects the permittivity, which changes significantly during roasting, is temperature. An experiment was developed to observe the effect of temperature on the roasting system. It measured the roasted coffee while it cooled at the end of a coffee roast. At the end of a coffee roast, most of the coffee's moisture should have been boiled off and the coffee will also stop roasting, so should be chemically static.

The plot in Figure 42 shows several measurements taken at different temperatures while a roast of Costa Rican Arabica was cooling down. Initially at a high temperature the peak was attenuated and had a lower frequency but as the coffee cooled down, the peak grew and frequency increased. Coffee at a high temperature has a similar effect to having a coffee with more moisture.

These sets of measurements (Figure 40,Figure 42) were used to understand the relationship between permittivity and the of the characteristics of the resonant peak. These measurements show that an increase in temperature or moisture equates to an increase in absolute permittivity. It can be said that for this system an increase in permittivity will cause a decrease in resonant peak amplitude and frequency.

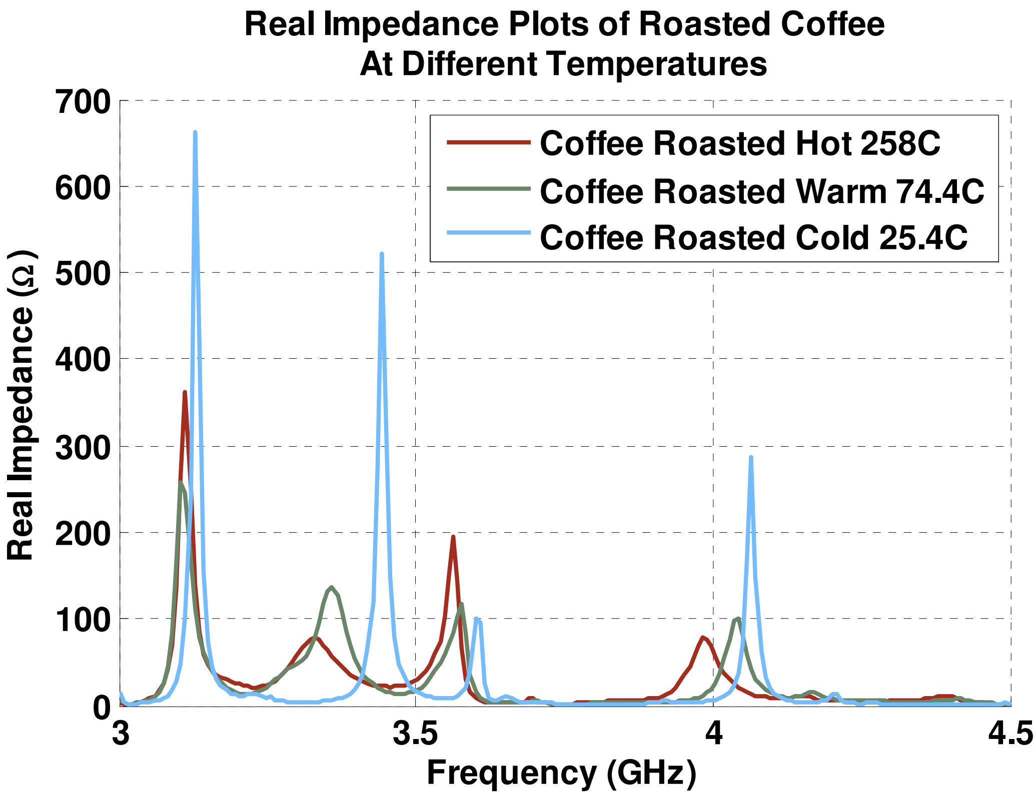


Figure 42. Comparison of Z-real plots taken on a load of coffee at different temperatures.

5.6 Allowing for the Movement of the Coffee Beans

At this point the relationship of the coffees moisture and temperature to the resonant peaks is quite well understood. However, understanding that relationship without a method of reliably tracking the resonant peaks through the roast was not useful until the movement could be accounted for. Figure 43 shows a measurement taken from green coffee. There was a marked increase in the variation of the measurements when the beans started to move. This became worse as the roast progressed, because the coffee bean’s density decreased. The bean movement therefore increased, making the variation worse. The problem then became how to make useful online measurements of the coffee.

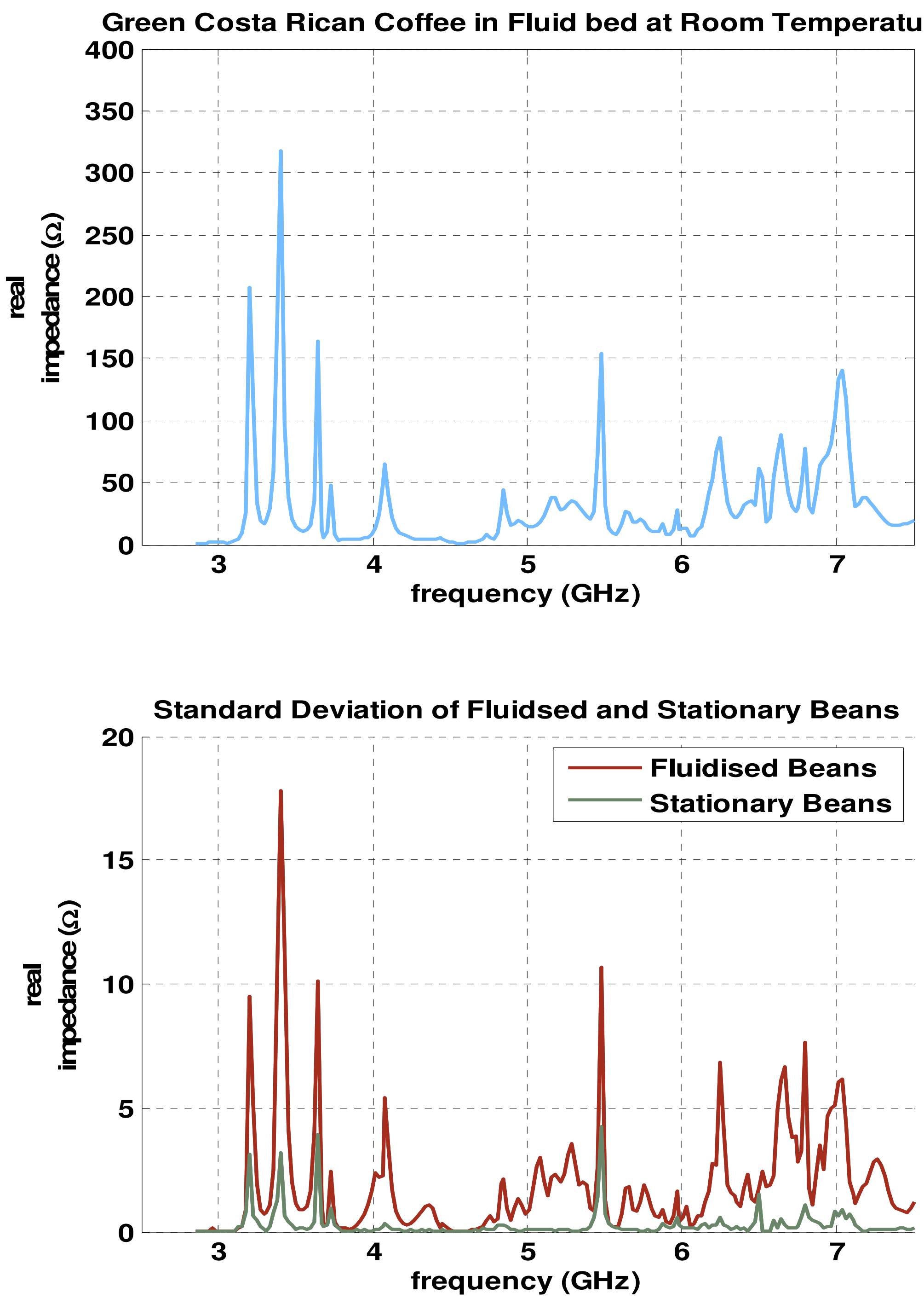


Figure 43. Z-real measurement of green coffee averaged over multiple sweeps (top), standard deviation of each point in different conditions (bottom). The figure illustrates the effect the motion of the coffee beans have on this method of measurement.

5.6.1 Possible Solutions

There are three possible approaches to solving the problem: 1) changing the roasting method, 2) putting pauses in the airflow, and 3) creating a method of getting useful data out of live roasts. Another roasting method was considered, however, all methods of coffee roasting require the beans be agitated to produce an even roast. This means that whatever the roast method, the problem of movement noise will remain. So, changing the process would likely have been fruitless.

Also considered, and tested, was taking measurements during roasting while the fan was temporarily paused. This method did return better, less noisy, results (Figure 44 and Figure 47). However, it had some short comings.

The first problem was that pausing the fan during the roast caused a temperature drop in the coffee. This meant that the results would skew from what was occurring in the coffee during standard roasting. The temperature dip also added an element of randomness to the roast, reducing the probability that two roasts would match, thus making repeat testing difficult. Figure 44 shows the temperature measurements taken from a roast attempted using this approach.

The second problem was one of response time. Taking pauses temporarily stopped the roast, and created discrete data points. This removed the real-time feedback on the condition of the roast. Although data could be used to show how the roast had progressed, it couldn't show the rapid changes in the data or display transient spikes. In the end this approach was not used because it didn't allow for the observation of transients.

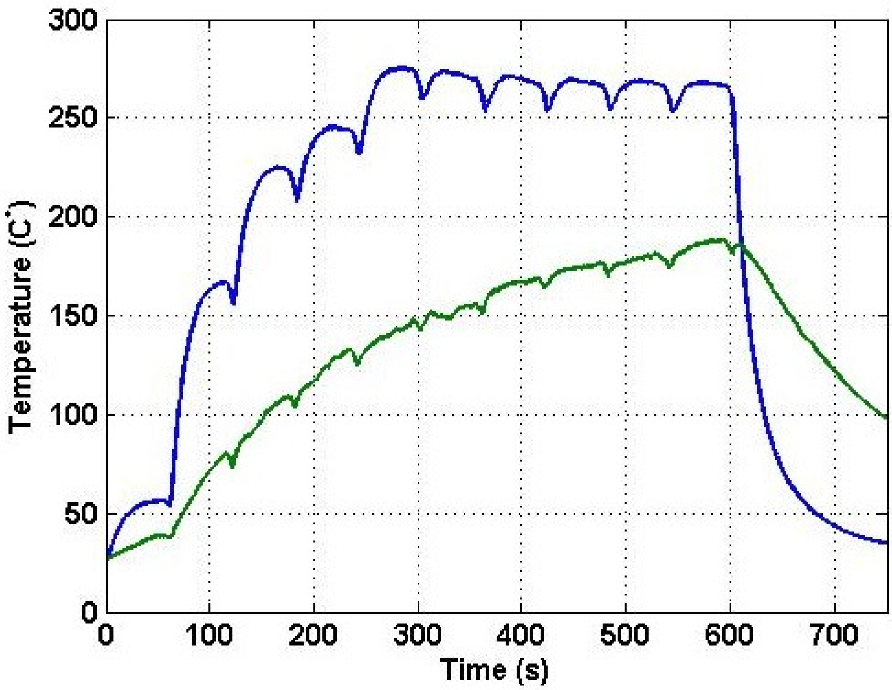


Figure 44 Input and output temperatures from a roast where the fan was stopped briefly every minute to take a microwave reading.

5.6.2 Making Sense of the Movement Noise

The solution was to observe a roasts worth of data stacked as a 2D image rather than discreetly trace by trace (Illustrated in Figure 45). By stacking the sequential traces into an array the roast progression could be displayed as an image. An example image (Figure 46) shows a roast worth of Z-real stacked up and displayed as an image. The frequency is displayed in the vertical axis, time in quarter second intervals on the horizontal, and the impedance is shown in the intensity. Storing the traces in this way helped with visualising what was happening and allowed the use of image processing techniques to find and track patterns in the data.

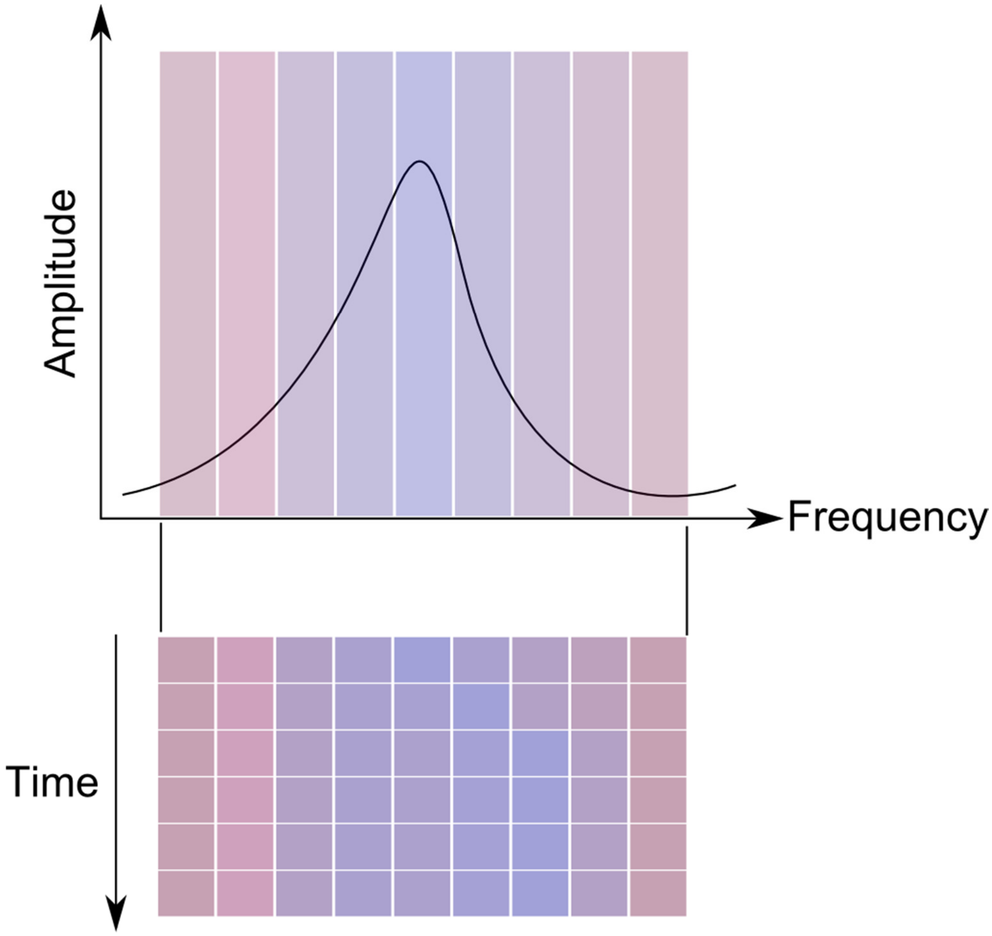


Figure 45 Illustration of converting network measurements into an image. The discrete values from the original measurement are sequentially stacked into an array.

This approach works well with programming environments that store and deal with data in matrices such as MATLAB. Using MATLAB, data from the network analyser is stored in a matrix. The matrix's rows represent frequency and columns the sequential measurements. MATLAB's built-in functions —such as *image()* or *imshow()*— can then be use to display the data as an image.

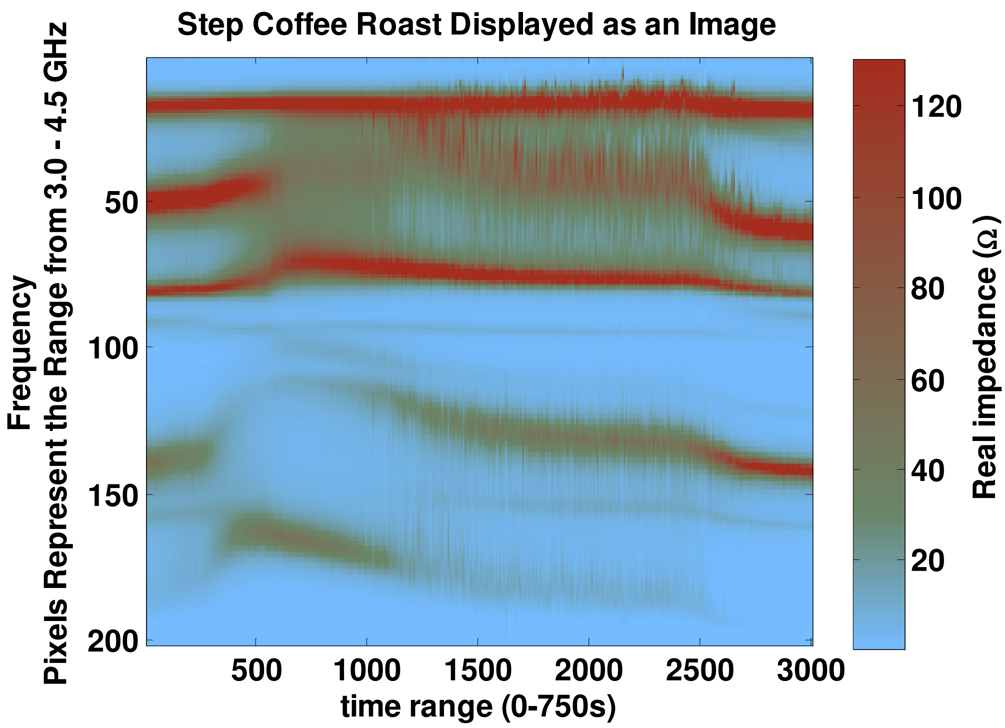


Figure 46. Image representation of Z-real; the data was produced in a standard step coffee roast. Each pixel contains an impedance value. Sequential frequency sweeps layered to produce an image that shows the change in Z-real with time. The pixels (in this case from 1-201) represent the discrete frequency measurements with the 1st pixel representing the low frequency (3GHz) and the 201st the high frequency (4.5GHz).

As an aside, a second example of a roast's network analyser measurements in image format is seen in Figure 47. This data is taken from a roast where the fan has been paused every minute (as discussed previously). In this example, the fan stopping adds a very visible transient every minute (approximately every 240 horizontal pixels). What can be noted from this example is that the effect of stopping the fan is pronounced in the latter half of the roast. This is when the beans are less dense and therefore moving more quickly. Also, the sections where the fan is stopped are on average higher in frequency then their surrounding moving sections.

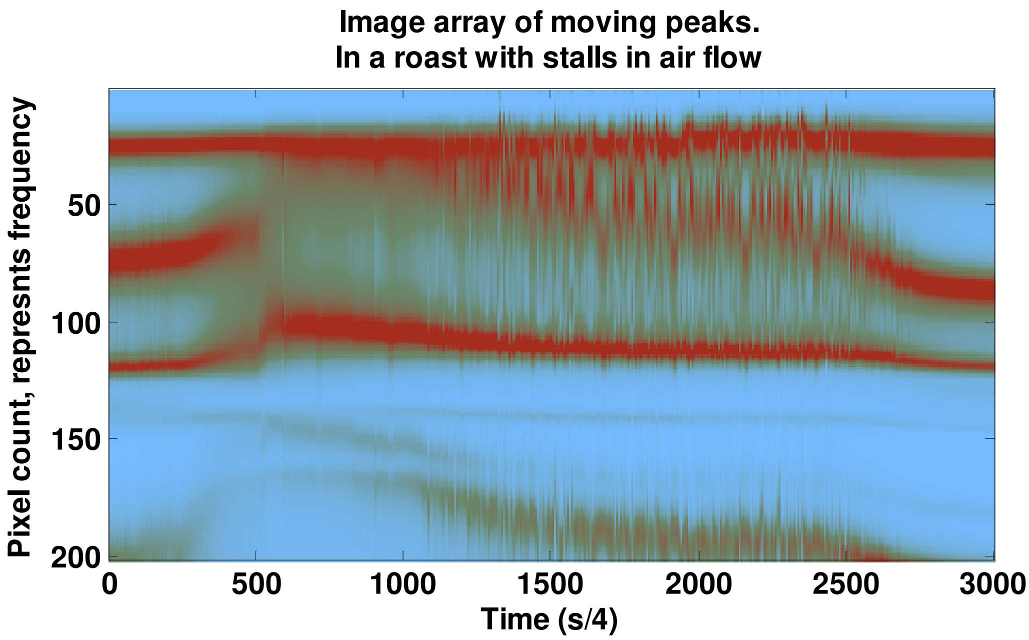


Figure 47. The network analyser measurements from the roast with fan pauses (temperature traces in Figure 44)

5.6.2.1 Reducing the Frequency Window

Looking at the data in this format (Figure 48) the resonant peak that moves between 3.2 and 3.5GHz becomes unsuitable for use. This is because in the early to middle section of the roast it overlaps with a surrounding peak. There was another resonant peak around 4.0GHz (initial pixel count around 140 in Figure 46) that followed the same patterns as the larger 3.5GHz (initial pixel count around 50 in Figure 46) peak and was isolated from other surrounding peaks. Having chosen the 4.0GHz peak, the region of interest was reduced to cover the range the peak moved over the course of a roast (Figure 49). The next step in tracking the peak was reducing the movement noise.

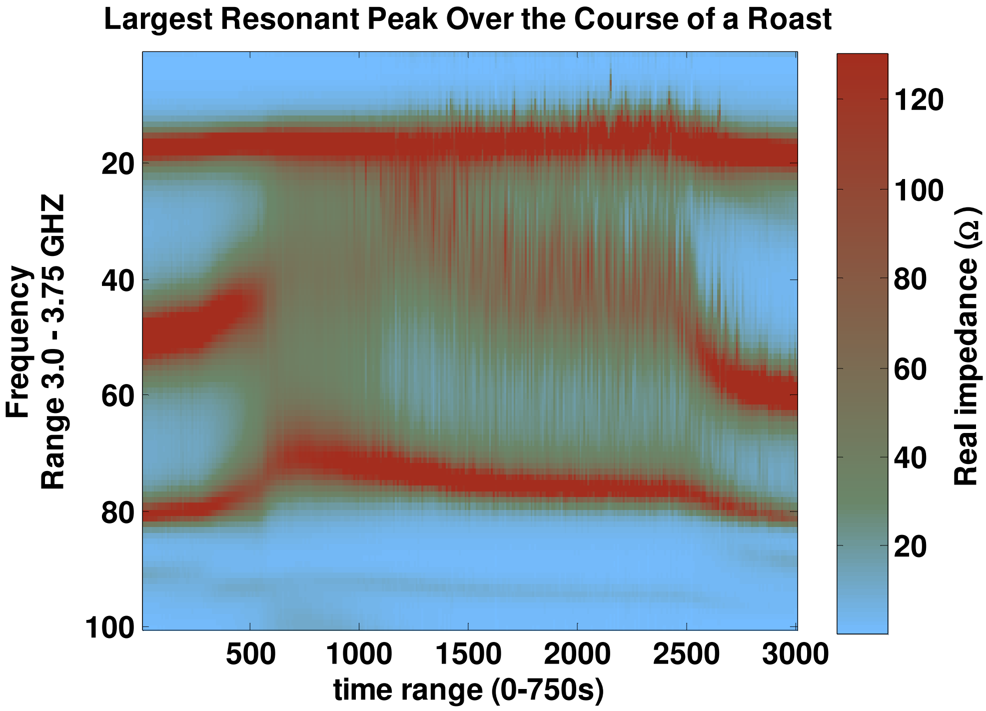


Figure 48. Image representation of the largest resonant peak, data collected from a standard coffee step coffee roast. It shows the peak getting lost in the movement noise and overlapping with its peaks surrounding peaks.

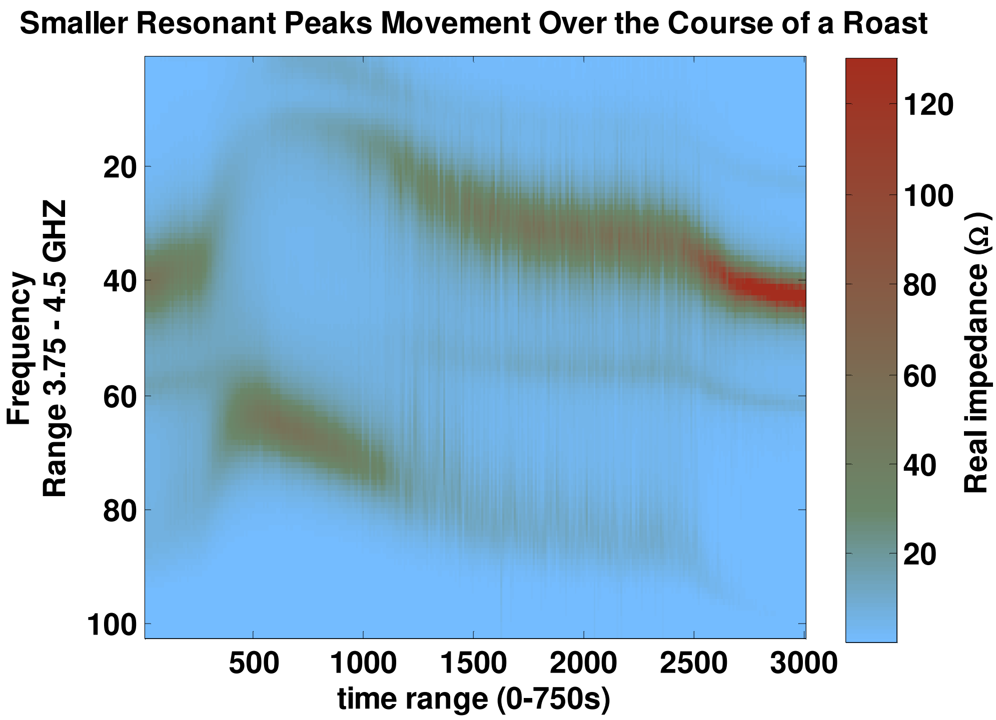
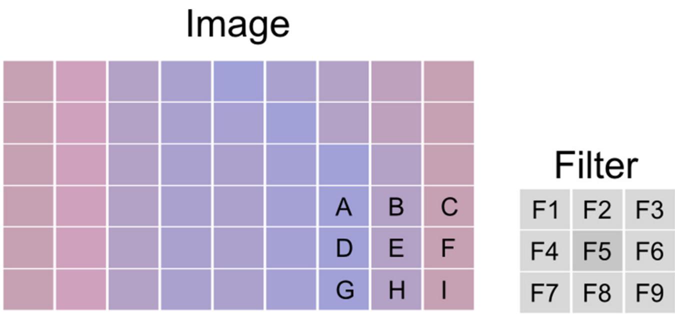


Figure 49. Image representation of a smaller resonant peak. The data was collected from a standard coffee step coffee roast. This peak, although smaller is not as susceptible to movement noise and has no surrounding peaks to be lost in.

5.6.2.2 Peak detection and tracking

A series of filters both in frequency and time were used to reduce noise and make it possible to track the peaks through the roast. Typical image processing filters are 2D (Illustrated in Figure 50). 1D filtering is done the same way as 2D but with a 1-by-n filtering matrix. 1D filtering is used in this case to make the technique more applicable to real time measurement. Temporal 1D filtering using a filter matrix whose values are all 1 is a form of low pass filtering and behaves the same as a running average would.

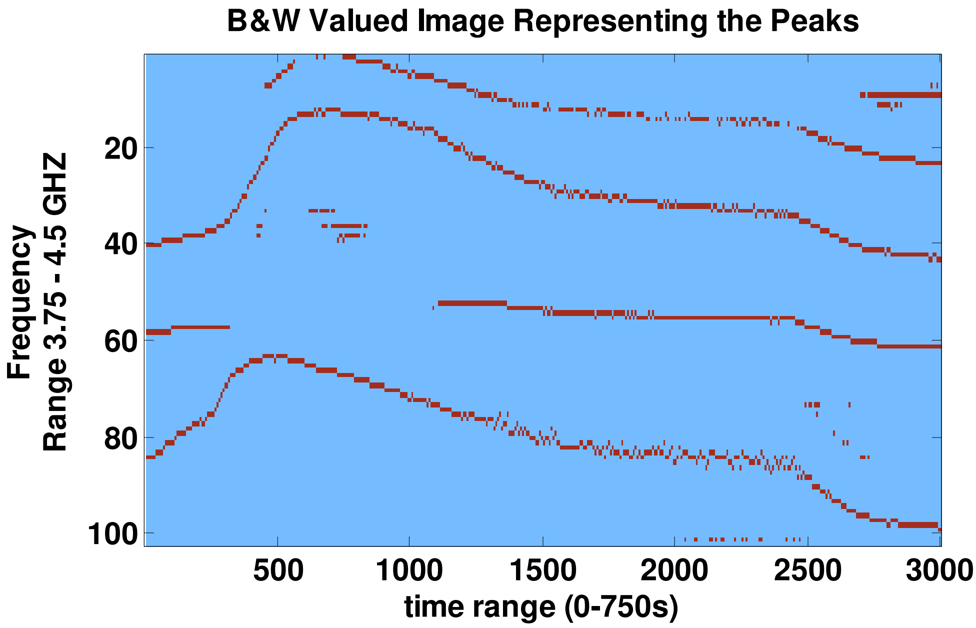
For this experiment, low pass 1D filtering methods were used in both dimensions separately. This means that the filtered result retains the structure of the original data but reduces the effect of movement noise. The filtered data allowed for the isolation and tracking of the peaks. Filtering was done using the MATLAB 1-D filtering function, *filter()*, and used a 1-by-5 filter array, repeated multiple times.



$$E = \frac{(F1.A+F2.B+F3.C+F4.D+F5.E+F6.F+F7.G+F8.H+F9.I)}{\text{number of pixels in filter}}$$

Figure 50 Illustration of a 2D image filtering method. For a given pixel (E in the case of this illustration) the surrounding pixels are multiplied pixel by pixel against a filter matrix. The original pixel is replaced by average value of this result. The behaviour of the filter is defined by the size, shape, and values in the filter matrix.

A stock MATLAB peak detection function (*findpeaks()*) was used to find all the peaks from the filtered data in the frequency dimension. This produced a black and white (or binary) image — shown in Figure 51 — that represents all the peaks from in the frequency window. Another function was used to further reduce the peaks down to just the peak of interest.



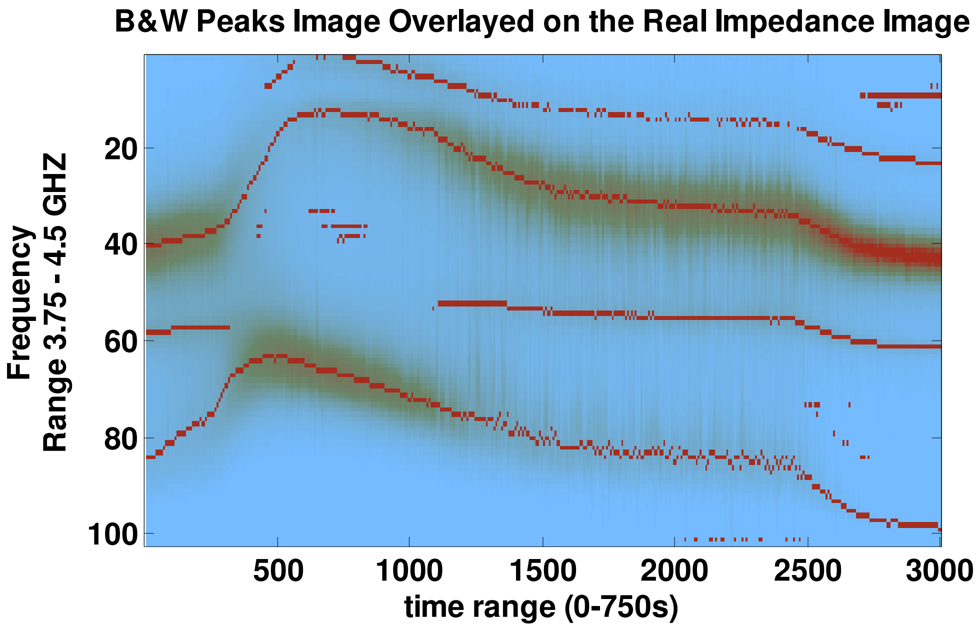


Figure 51. Binary image showing the peaks and their progression through the roast (top). Binary image overlaid on the Z-real image (bottom).

The function's job was to remove the extraneous peaks from the black and white image. There are several ways to do this. The first would be to define the starting frequency and have the function find the closest peak in the next sweep and continue through until the end of the roast. This method is what would be applied in a real time online setting.

As the data could be post processed, black and white image processing techniques could be used to isolate the main frequency. The process was to fill the image (using *imdilate()*, a basic example of this is shown in Figure 52), label the various white sections (using *bwlabeln()*), find the largest group and remove the others, then finally un-fill the image (using *imerode()*, example in Figure 53) leaving the single main trace. This process produced a single time vs frequency resonant peak (Figure 54).

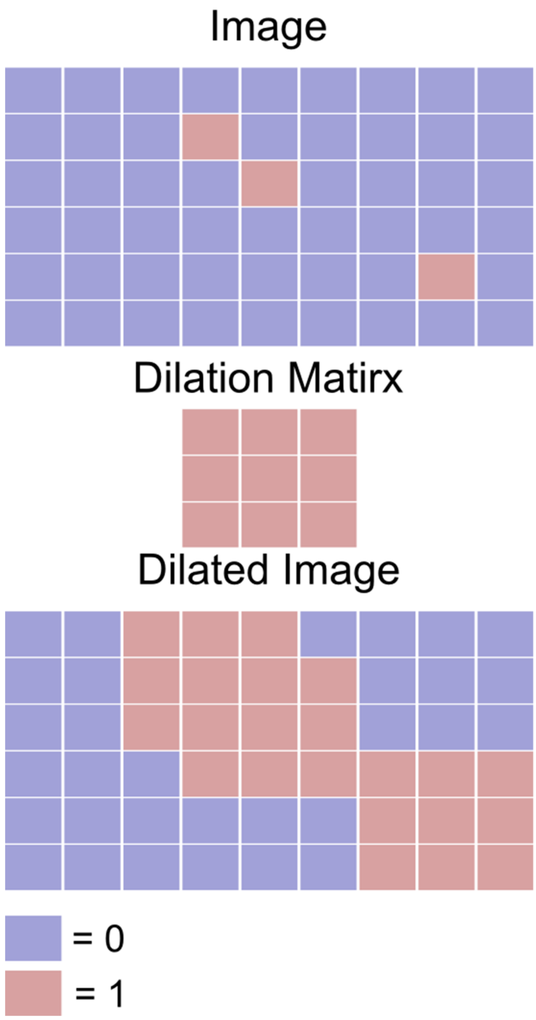


Figure 52. Binary image dilation illustration

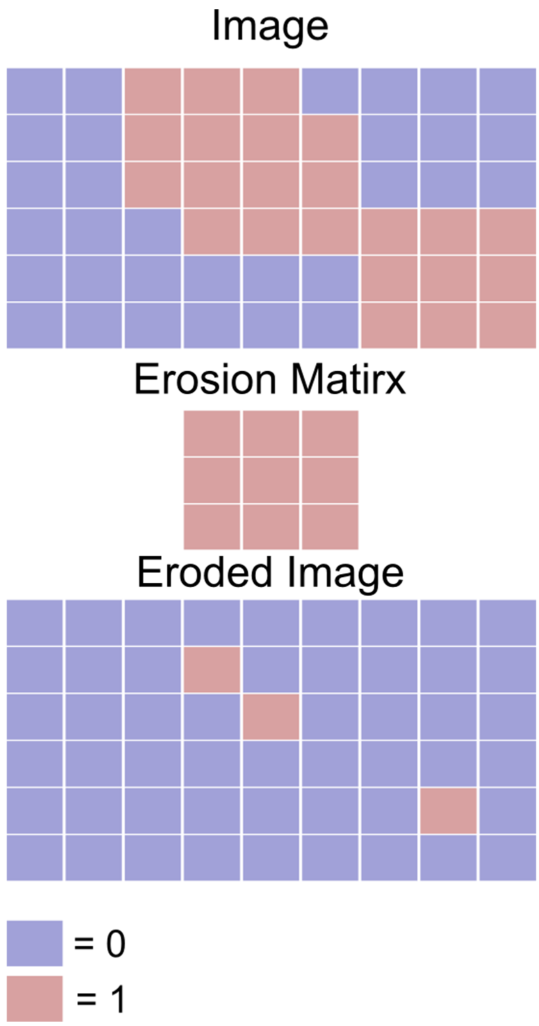


Figure 53. Binary image erosion illustration

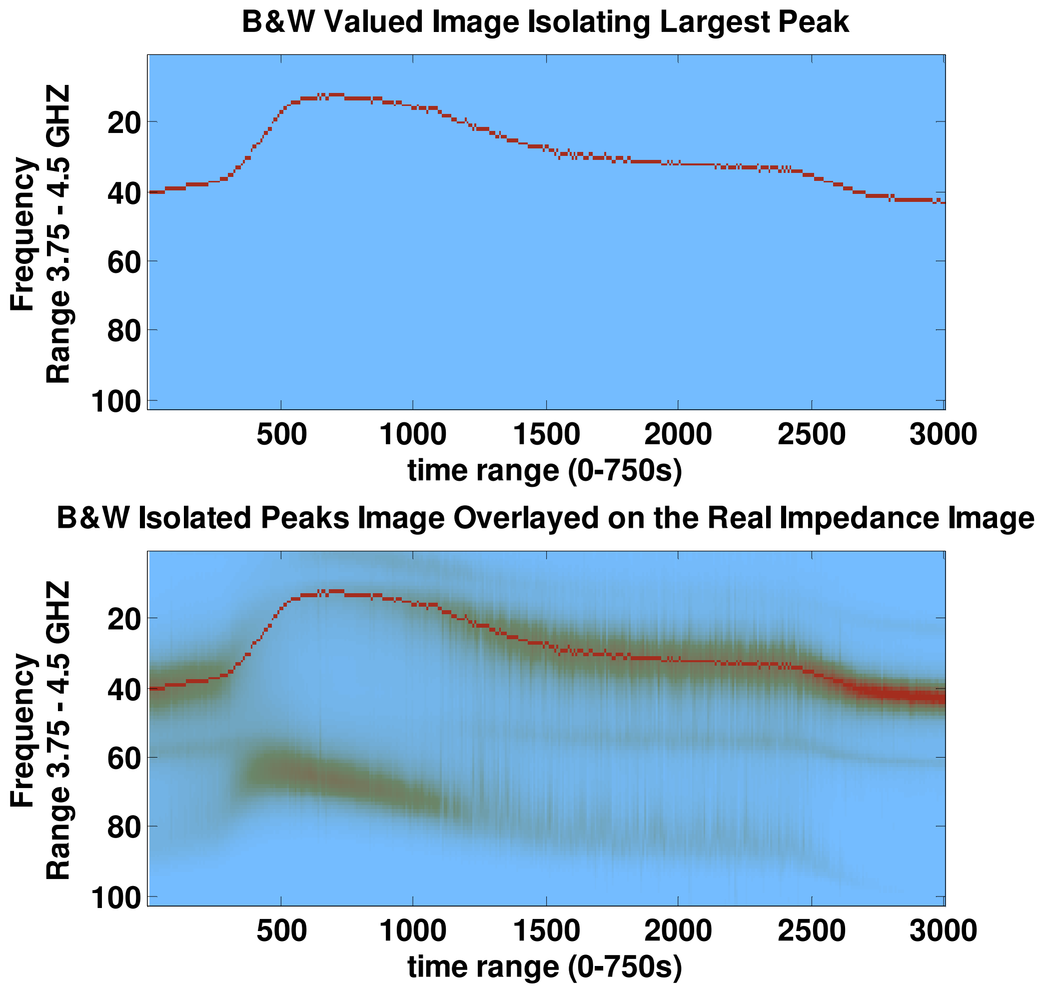


Figure 54. Binary image of the single largest –and therefore most consistent- peak tracked through the roast (top). Binary image overlaid on the Z-real image (bottom).

5.6.3 Result

The result is a process that can automatically isolate the resonant peak of interest —as it moves through the roast— from the noisy data. Figure 55 shows two different temperature profile coffee roasts processed with this method. The peak has been isolated in each of them. Observing both the frequency and amplitude of the peak showed that they both followed similar patterns. The amplitude however was noisier. Additionally, it was reliant on the isolation technique to locate the peak. This meant that it would sometimes show the wrong value (Figure 57 Comparison in tracked peak's shift in both frequency and amplitude). For reliability and consistency subsequent conclusions are drawn from only the frequency information.

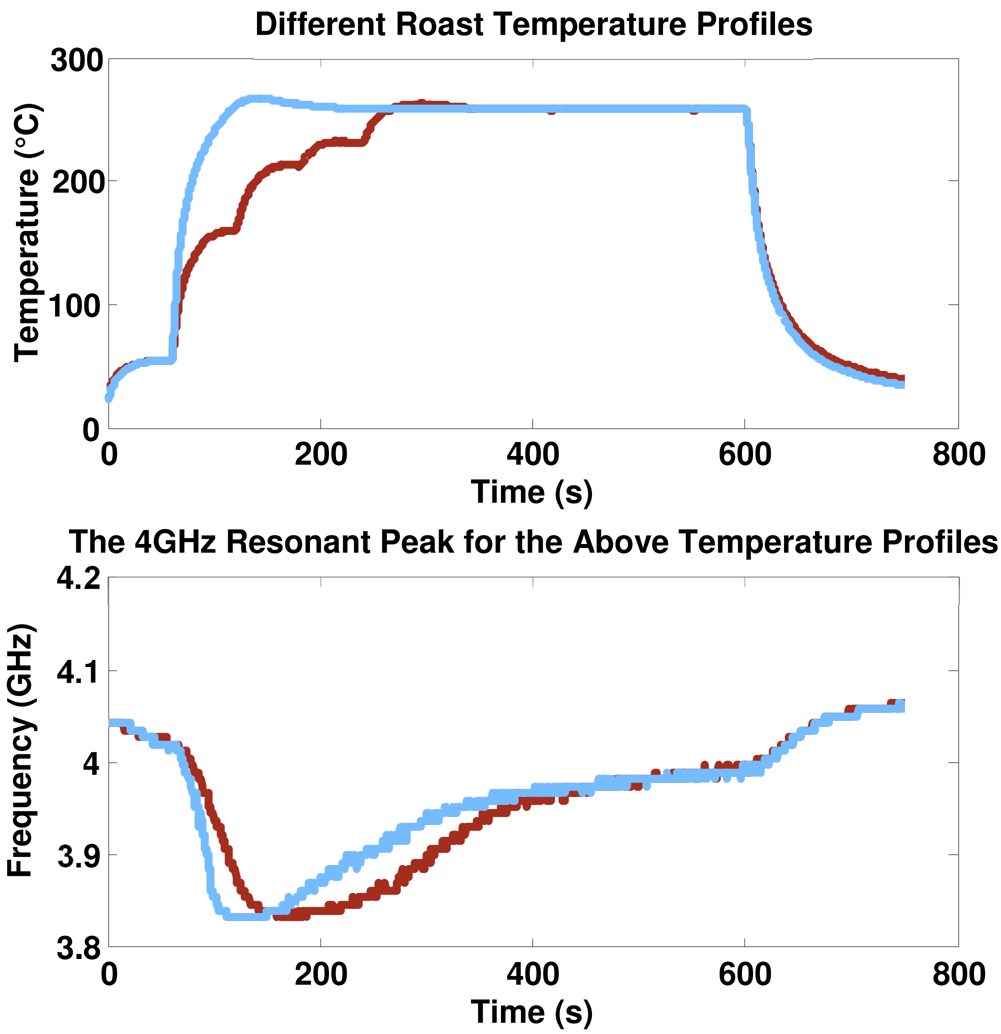


Figure 55. Two different step coffee roast temperature profiles (top). Corresponding resonant peak measurements (bottom).

5.7 Observing the Changes in a Coffee Roast

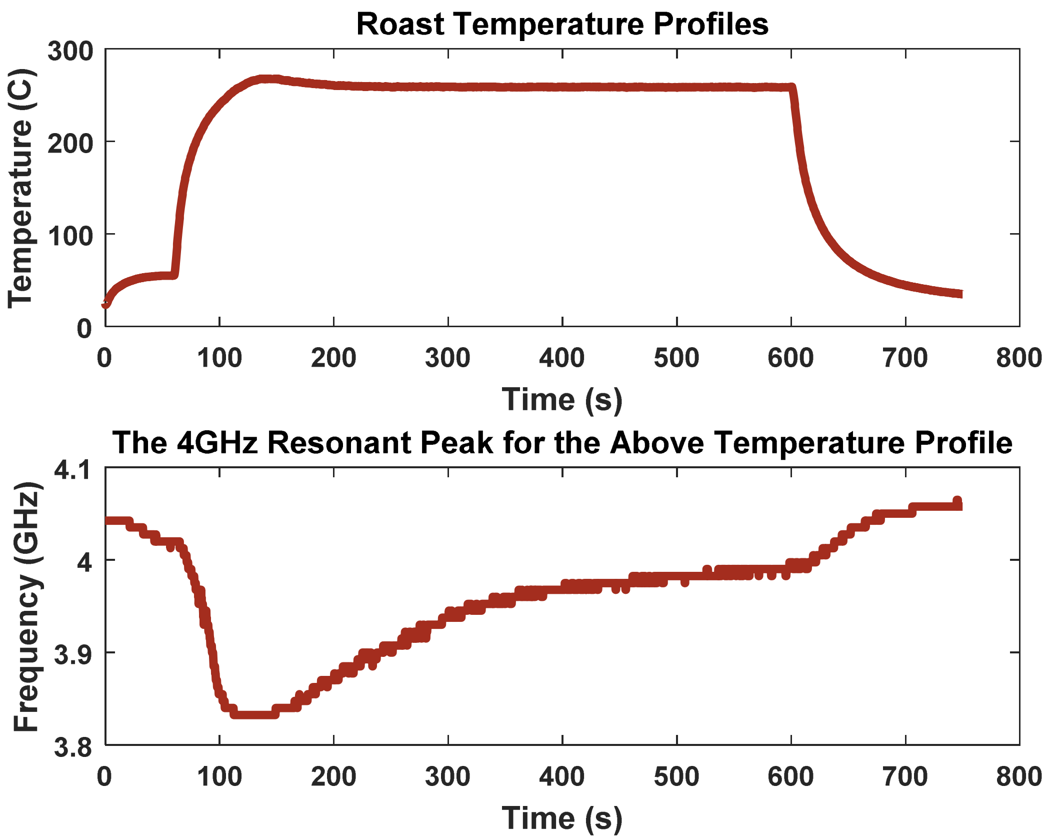


Figure 56(top) shows the temperature roast profile of a straight step. Applying the resonant peak isolation technique to data measured from a roast with the straight step temperature profile produced

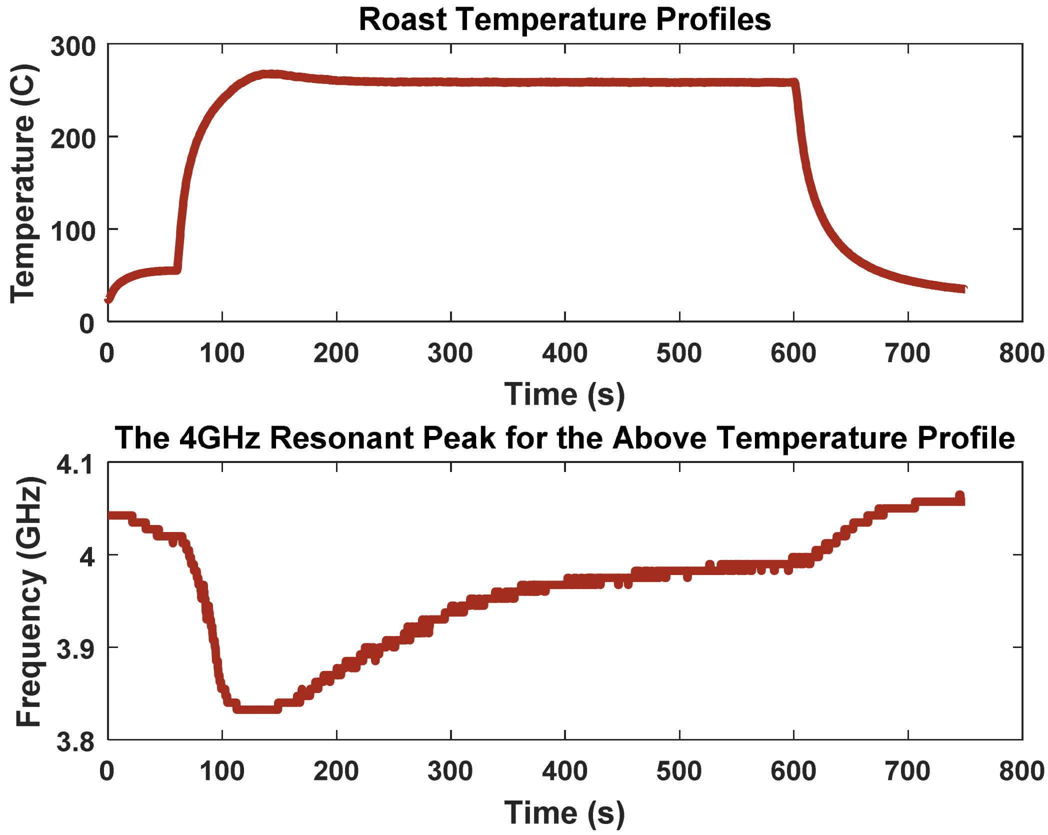


Figure 56(bottom). Conclusions can be drawn, about the changes occurring in the coffee during roasting, using this measurement and the information obtained on how moisture and temperature affect the measured peaks.

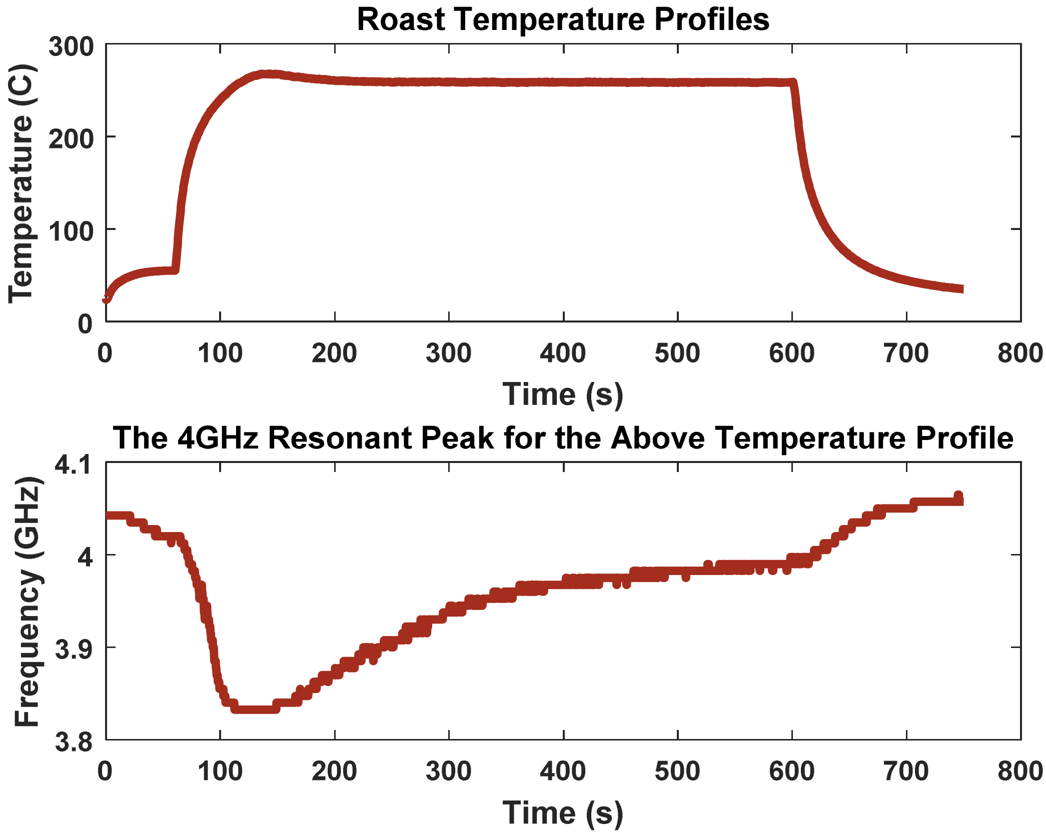


Figure 56. Resulting microwave resonant peak measurement (bottom) and temperature profile (top).

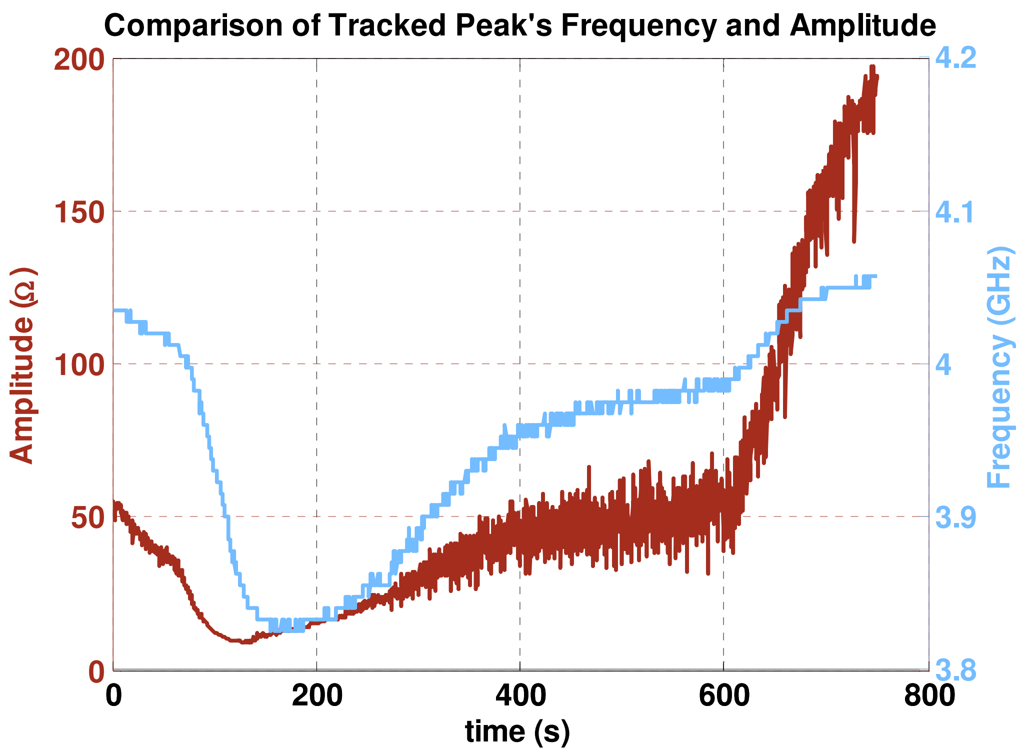


Figure 57 Comparison in tracked peak's shift in both frequency and amplitude

5.7.1 What is Observed from the Coffee Roast?

What is observed is the change in temperature and the change in moisture working against each other. The large initial temperature increase causes a rise in permittivity, lowering the peak's frequency. As the coffee heats up it starts to lose moisture causing a loss in permittivity, increasing the peak's frequency. As the temperature increases, the rate of moisture loss also increases. Before the temperature peaks, the moisture loss overcomes the temperature increase and the peak starts shifting back. For the second portion of the roast (in the region of interest) the temperature has levelled off and it is observed that the peak increases in frequency. This increase can be attributed to the coffee beans' continued loss in moisture.

These measurements are consistent with what was expected from roasting coffee and align with our pre-test measurements. The measurement does not show any definitive transients. This meant that it could not be used for the detection of the ideal end of roast time.

5.8 Fitting to the Thermal Model

A method of clarifying results was to compare the data from the microwave measurement to that of the thermal model. The question being, does the moisture measurement match with what was expected in the thermal model? Ideally the loss in moisture predicted by the model will behave like that of the moving resonant peak; showing that they are observing the same thing.

To do this the thermal model was modified to work with the measurements from the stainless-steel roasting chamber. This was achieved by building a thermal model of the empty stainless-steel chamber in the same way as the model was made for the glass roasting chamber. This model was then combined with the model of the coffee created in the previous chapter. The functional result is shown in Figure 58.

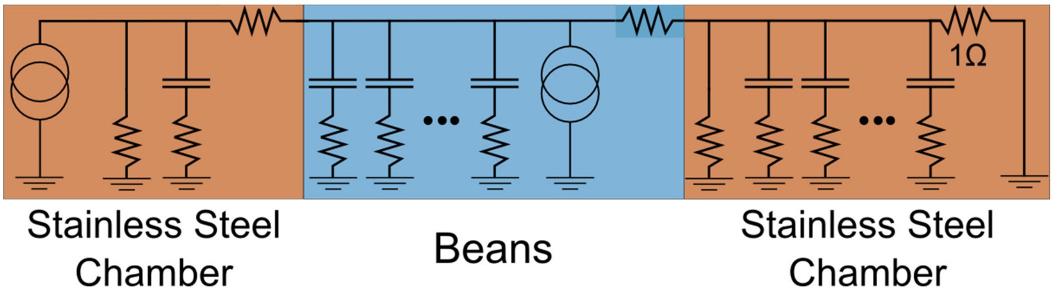


Figure 58. Layout of thermal model modified to work with stainless steel roasting chamber. The stainless-steel section was modeled empty and the bean model was taken from previous measurements.

Applying this method produced the result seen in Figure 59. This shows that in the case of the measured results the chamber loses much more heat than the model predicts. Although the shape of the model generally matches that of the measured data there is still a large discrepancy. This result highlights the differences between the glass roasting chamber and the stainless steel one.

The glass roasting chamber has a lower thermal mass, lower thermal conductivity and produced more thermally stable results than the stainless-steel chamber. Thus, the variation in the exhaust in the stainless chamber is significantly larger than the glass chamber (Figure 60). Therefore, it is unsurprising that the model didn't fit as well, because the model works out a more ideal scenario.

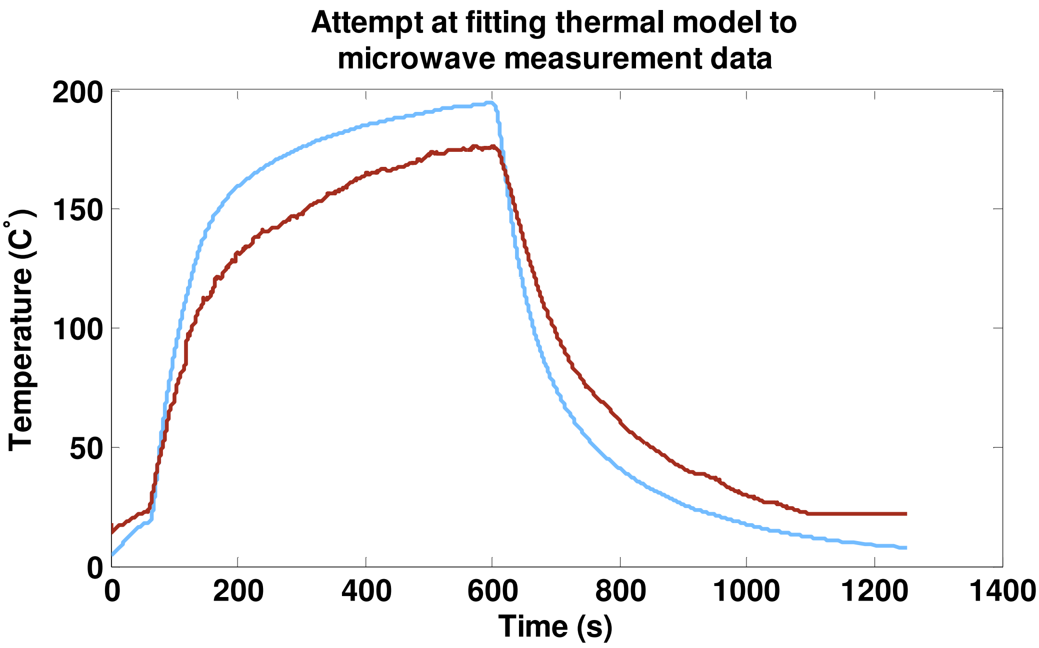


Figure 59. Initial model fitting. The model prediction and the result have similar shapes but have around 30 °C in error at their worst.

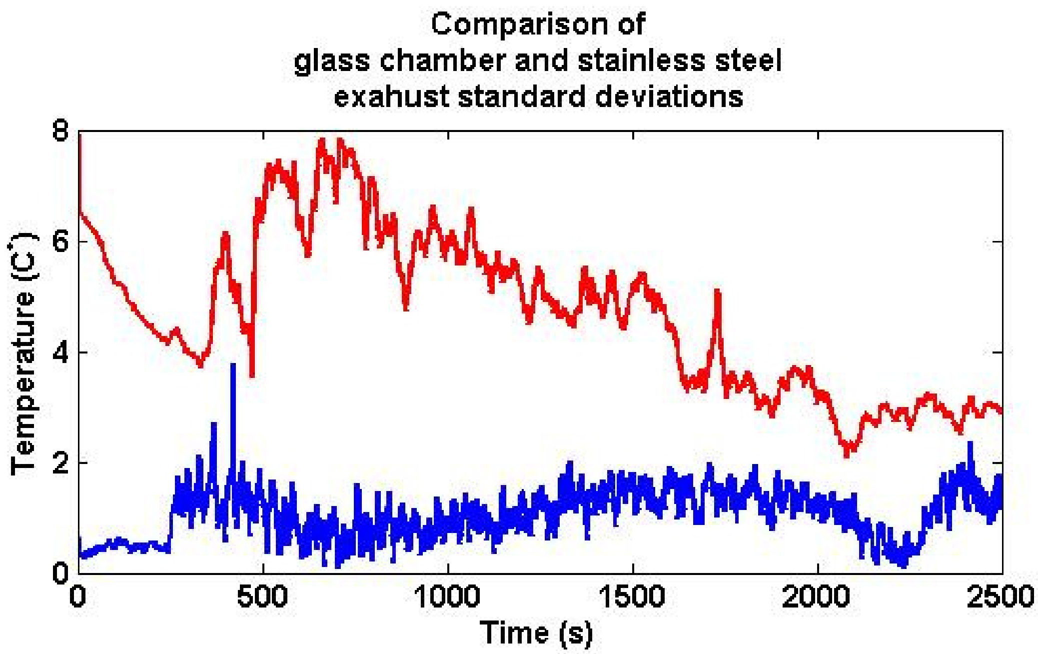
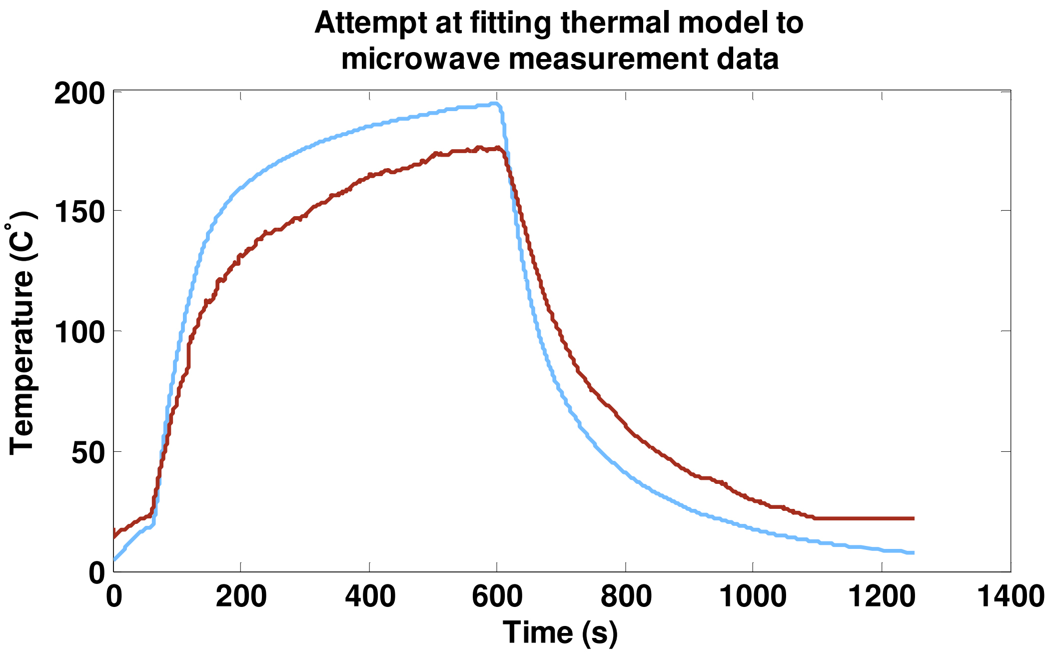


Figure 60. Difference in standard deviation of exhaust profiles over multiple roasts. Comparing the stainless-steel (Red) to the glass roasting chamber (Blue). The glass chamber is shown to have a more consistent exhaust.

It was possible to change the model of the stainless-steel section to create a better fit to the real data. Increasing the capacitance of the model to emulate the loss of heat out of the chamber and Figure 60 was produced. This was an improvement that is suitable to make some comparisons from.

In Figure 62 the movement of the network analyser peak is compared to the modelled bean moisture. Both sets of data are scaled to be a percentage of their respective maximums and minimums. Even though they are not a perfect fit, they do both follow the same descent pattern as the roast progresses. This shared descent further reinforces the idea that the peak movement measured by the network analyser is the loss of moisture from the roasting coffee.



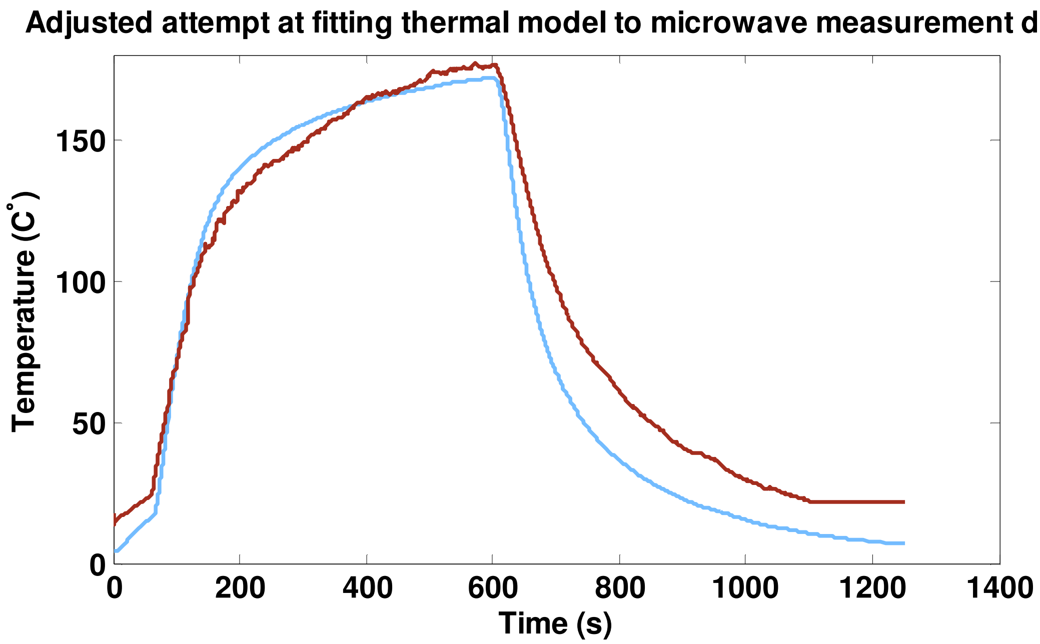


Figure 61. Model with adjusted to create best fit with measured data.

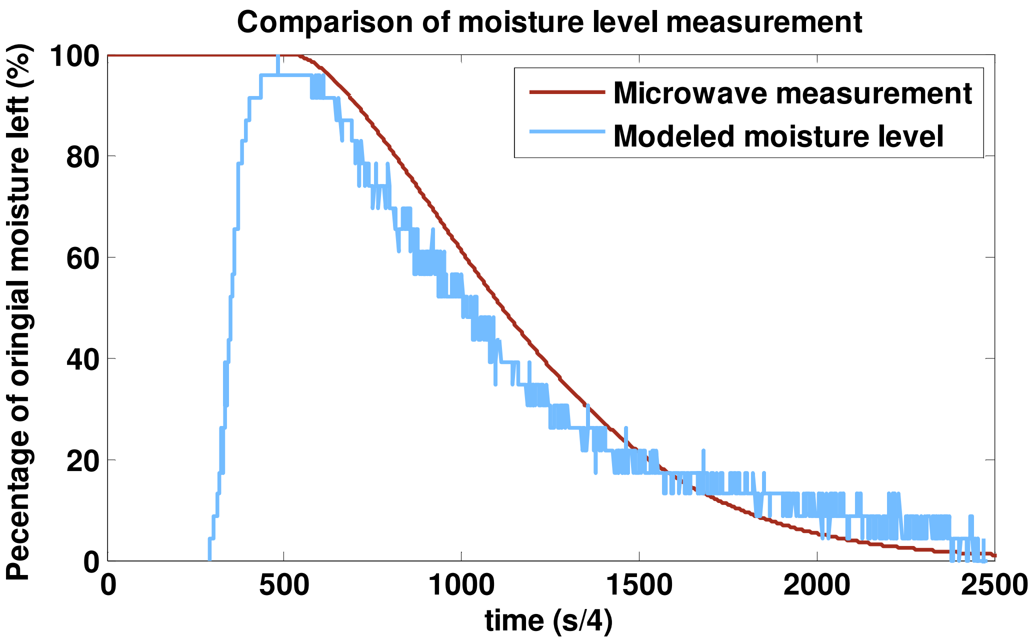


Figure 62. Microwave measurement compared to thermal model of moisture level.

5.9 Conclusions

In this chapter, the use of a microwave frequency measurement of coffee in real time as it roasted was investigated. This required the construction of a unique roasting chamber to make the measurements. The method of measurement was a single port resonant cavity. The effects of both moisture and temperature on resonant peaks of the cavity were measured. Then the coffee was roasted and the effect on the same resonant peaks observed.

The coffee roast was found to have a lot of noise created by the mechanical movement of the coffee beans. This mechanical noise created an overlap in the largest resonant peaks, causing them to be lost in the noise. Smaller higher frequency peaks became the focus as they followed the same patterns as the larger, but were not lost in similar noise.

To isolate the movement of the chosen peak, a signal processing function was created. The data that returned from the function was analysed and interpreted in how it related to the changes that coffee experiences during roasting. It did not have any consistent transients or major inflections that could be used to identify the end of roast.

The stainless-steel roasting chamber was thermally modelled so that the results from the microwave measurements could be compared to the thermal measurements from a glass chamber. The stainless-steel roasting chamber was very poor for thermal measurement. Therefore, a direct comparison model didn’t fit the measured data well. The model could be adjusted to create a better but not perfect fit. With the modified model a comparison could be made between the network analysers moisture loss result and thermal models modelled moisture. It is not a perfect fit but the model shows agreement to the measured data.

The measurements made in this chapter are interesting because the progression of the roast can be tracked online as the coffee roasts. This method also found a solution to the noise problem created by the mechanical movement of the coffee in the fluid bed. It produced a plot of the frequency peaks movement during the roast. However, it did not reveal any major waypoints or transients during roasting that would predict the ideal roast end. The mechanical movement solution could be used in the future in a method that identifies the ideal roast end via a series of different measurements.

6 Application of Raman Spectrometry

6.1 Chapter Summary

The search for end of roast indicators have so far covered the thermal analysis and moisture loss of coffee as it roasts. These trials produced interesting results but didn't have a transient or defined signal that could be used as a direct indication of roast completeness. This chapter moves on to looking at the changing surface chemistry of the coffee.

The changing chemistry in coffee roasting is physically obvious with the dramatic colour change that occurs during roasting [37]. This chapter discusses the use of a Raman spectrometer to make online measurements of the changing surface chemistry of coffee.

Initial testing involved making offline measurements on single coffee beans. The beans were prepared by roasting batches using a set temperature profile for different lengths of time. Several beans from each of the batches were measured in the Raman Spectrometer. The results showed that the Raman spectra were drowned out by increasingly intense fluorescence. However, the fluorescence did increase in overall amplitude with roast progression. This changed the focus from looking at Ramen spectra to seeing if roast progression could be measured with fluorescence. In general, the fluorescence increased as the bean got darker and more roasted. Also, fluorescence was dependant on the spectrometer's focus and position on the bean. This caused some overlap in fluorescence between discrete samples. Closer inspection of the fluorescence also showed that the there was no change in the small high frequency signal that was independent of the overall amplitude of this signal. This meant there was no Raman signal showing through the fluorescence. It also meant that there was no discernible transient displayed from the static tests.

The coffee roaster was modified so that it could make online roasting measurements with the Raman spectrometer's external probe. The external probe had a fixed focus point; this was set so that it focused on the coffee in the fluid bed. Repeated static tests had an inconsistent average fluorescence measurement. Taking a similar measurement on the coffee while it was fluidised returned a more consistent result.

The fluorescence measurements returned by the probe were all distorted by an unknown repeating distortion. The distortion could be characterised by looking at coffee roasted in discrete time steps and running a comparison between offline and online measurements in the fluid bed. Once characterised, the distortion could be removed from all subsequent results.

The results show a progressively increasing fluorescence with roast progression levelling off toward the end of the roast. The rate of increase slows toward the end of the roast. Ultimately, a repeatable transient that would signal end of roast was not detectable.

6.2 Applying Raman Spectrometry to Coffee Roasting

The goal of the experiment was to observe the changing surface chemistry of the coffee beans during the roast. This was attempted by using a Raman spectrometer. The Raman spectrometer that was used could produce real time results and had an external probe, allowing for online the measurement.

Raman spectroscopy has previously been applied to coffee as a method of distinguishing between green Arabica and Robusta coffees. To do this R. El-Abassy et al. [85] use a combination of Raman spectroscopy and principal component analysis. Their work focused on the determining the difference between two sets of static green coffee. El-Abassy's work is not directly applicable to this work as they are looking at different things, however they show that it is possible to get a functional measurement from the Raman of green coffee.

Raman spectroscopy has also been applied to make online measurements in a fluid bed. G. Walker et al. [86] submerged a Raman probe in a fluid bed of powder — as part of a pharmaceutical manufacturing process — to measure the various chemical concentrations of the moving particles. Their experiment allowed them to make a 3D map of the chemistry in their fluid bed. They did this by submerging the probe at various points in the bed and taking measurements. In this experiment it is not possible to do this because the high temperatures in the roast chamber would damage the probe.[13]

6.2.1 Introduction to Raman Spectrometry

The following section contains a summarised description of Raman scattering and Raman Spectrometry. For more detail, summaries can be found on the relevant wiki pages[88], [89], they are around 2600 words and 3500 words. Furthermore UC Davises has a chemistry wiki that contains good information about the theory[90] and application[91] of Raman spectrometry. For a more reputable source M.

[13] Infra-Red spectrometry has been used in a similar case to measure particles in a fluid-bed through a window see P. Findlay et al. [87].

Pelletier's book "*Analytical Applications of Raman Spectroscopy*"[92] covers the background, instrumentation, and use of Raman spectroscopy.

6.2.1.1 What is Raman Spectroscopy?

Raman spectroscopy is a method of determining a substance's chemical make up by observing the Raman scatter (also referred to as Raman Stokes scatter) of incident light. Raman scattering is the inelastic scattering of light. Most light that is absorbed by a substance is reemitted at the same energy (Rayleigh scattering) however a small percentage of the light reemitted loses some energy in the interaction; the result of which can be measured as a frequency shift. The size of the shift is determined by the quantum energy levels of the substance. By observing frequency shifts, extrapolations can be made about the makeup of the substance being observed.

6.2.1.2 Raman the practice of quantum theory

A Raman spectrometer shines a single frequency laser at a substance and observes the light returned. The laser excites the electrons on the surface of the substance and they increase to a higher energy level (illustrated in Figure 63). In most cases this energy level is a virtual energy level and is unstable, meaning that the electron immediately falls back to where it started and emits a photon of the same frequency (Rayleigh). In a small percentage of cases however the electron returns to an energy level different from where it started. In these cases, the frequency of the photon emitted is of a different frequency to the original. This can happen in one of two ways; the electron can fall to a state of higher energy than the original producing a lower frequency photon (Stokes scattering) or the electron can fall to a lower energy state from where it started producing a higher frequency photon (anti-Stokes scattering).

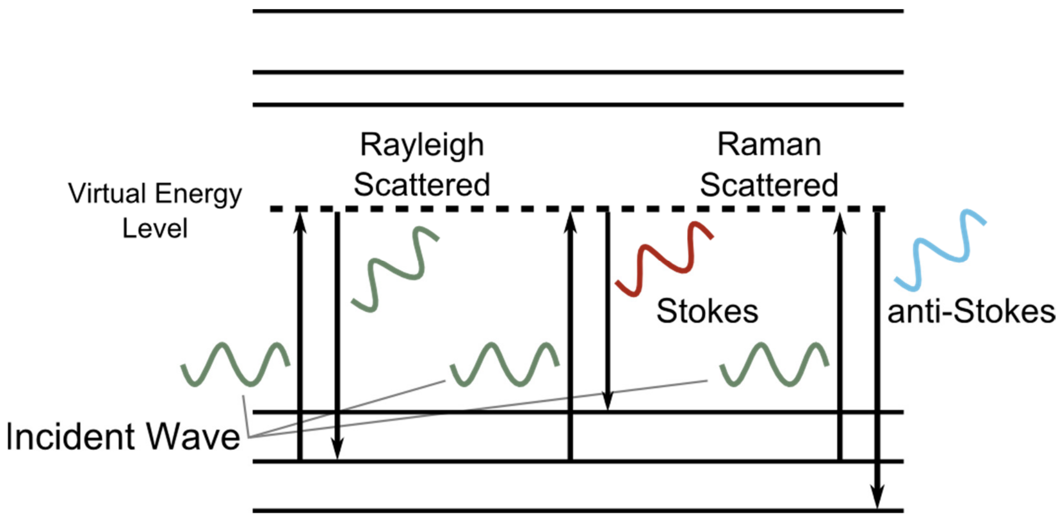


Figure 63. The sample's electrons are charged with an incident photon to a virtual energy state. When they fall from the virtual state they emit a photon. Most fall back to the initial level producing a photon of the energy (Rayleigh). Some however fall to a different level changing the frequency of the photon (Raman).

For the spectrometer to make a measurement on the Raman shift frequency it must filter out the Rayleigh frequency light which will be the majority of the returned light. The spectrometer then must split the filtered return into a frequency spectrum. This can be done using a prism or diffraction grating. The split spectrum is shone onto a light sensor. The light sensor such as a CCD can be a single point or line sensor. In the single point sensor case, the sensor or prism would be moved to scan the Raman shift spectra. The line sensor case means that the whole Raman shift spectrum can be acquired in a single capture. The PerkinElmer RmanFlex 400[93] used in these experiments uses something similar to the fixed line sensor method called echelle spectroscopy[94].

In this application, being able to take single capture spectra in combination with an external probe allows for the taking of sequential online measurement of the coffee while it is roasting.

6.2.1.3 Special cases

There are some special cases in which Raman spectrometry doesn't behave as it is desired. These cases are resonance and fluorescence. In the case of resonance, the incident light raises the electron energy to a stable level. Electrons that are raised in this way exhibit increased Raman scattering. There are methods of Raman spectroscopy that uses resonance to make measurements.

Fluoresce is caused when light is not scattered but absorbed by the sample and then readmitted. Fluoresce is a problem for Raman Spectrometry because it can be orders of magnitude bigger than the Raman scattered light, and it has a longer lifetime than Raman signals. Practically, this drowns out any actual Raman signal with what looks like broad band noise.

6.3 Preliminarily Testing

Initial Raman tests were on static single beans measured in the Raman spectrometer on its translation state. This test was to see if there was anything that could be observed on the coffee in the controlled environment that could be applied to the up-scaled fluid-bed tests. It also allowed for familiarisation of the equipment and to help predict issues that may have arisen in the fluid bed test.

6.3.1 Single Bean Test

Coffee was roasted in a series of batches using the step temperature profile, Figure 64, for different time intervals. Selected at random, beans from each batch were measured. The beans were placed on the Raman spectrometer's translation stage and measured. Mechanically, this meant the measurements were made by moving a bean sample under a fixed head containing the Raman spectrometer's capture optics. The head was focused (using the Raman spectrometer's inbuilt visual feedback) onto the sample to ensure the greatest possible return. Laser power and exposure time settings were chosen to ensure that the Raman's sensor did not saturate when measuring any of the samples, these values were kept consistent across all measurements. A series of captures were taken over the surface of each coffee bean. This produced the Raman plots in Figure 65.

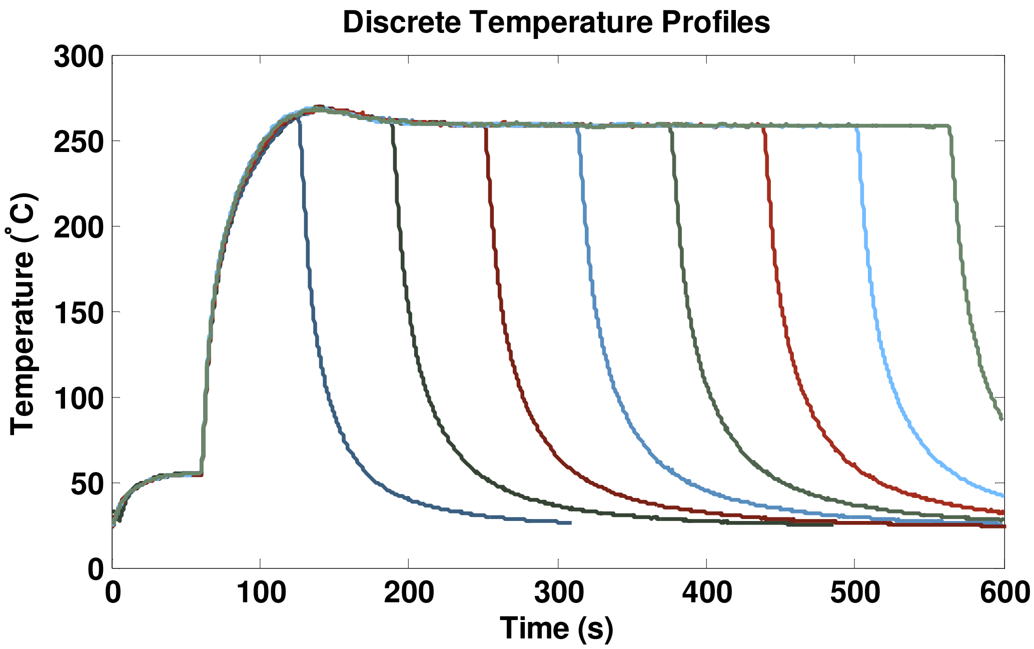


Figure 64. Set of different temperature profiles used for the measurement of coffee at discrete intervals during the roast.

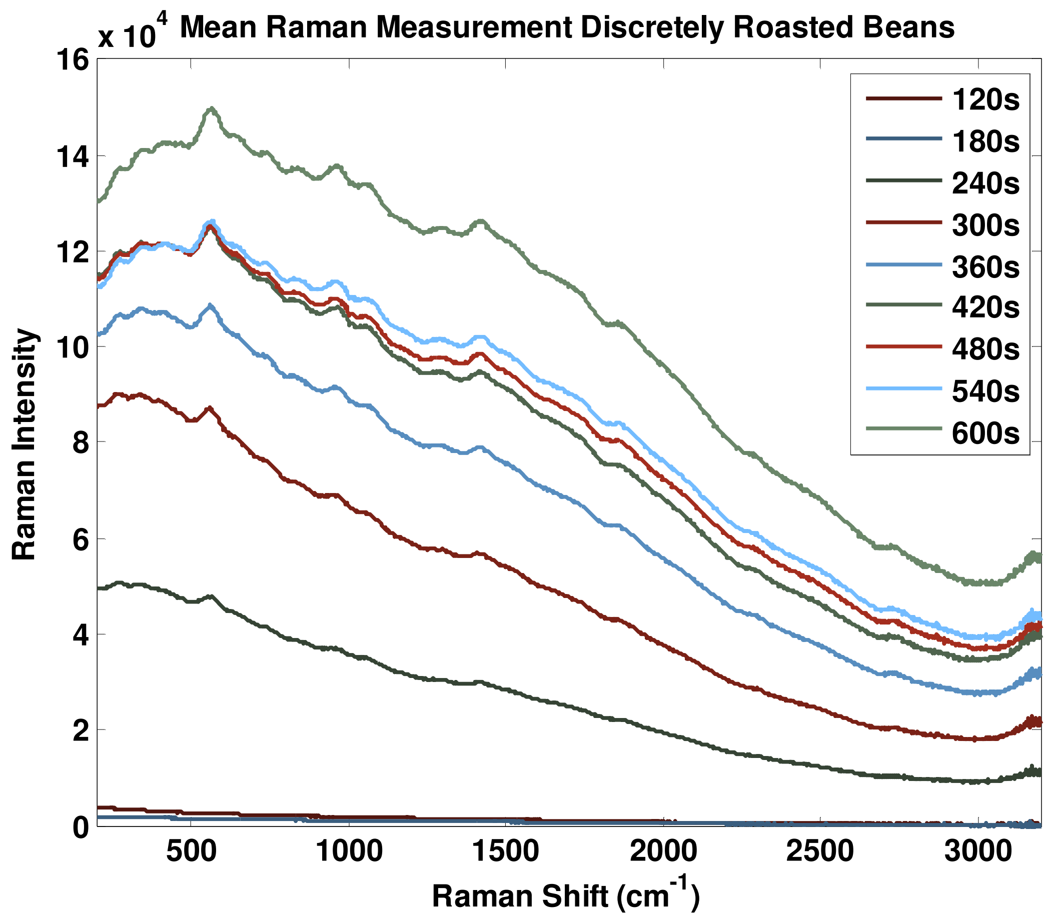


Figure 65. Mean of the Raman measurements taken from each set of discretely roasted coffee.

6.3.2 Single Bean Result Analysis

Figure 66 contains three sets of measurements. From this data, some initial observations were made, these include: the sets roasted for a longer time have a higher average value, there does not seem to be any frequency peaks that change with roast progression, and the sets are not perfectly clustered[14]. These observations prompted some additional questions. Is there any Raman scattering information in this data? Why are there, sometimes big, differences between signals taken on a same set of coffee? Can this result be used to signal roast completion?

[14] Notably these measurements of green coffee do not match what El-Abassy's measured in their examination of green coffee[85].

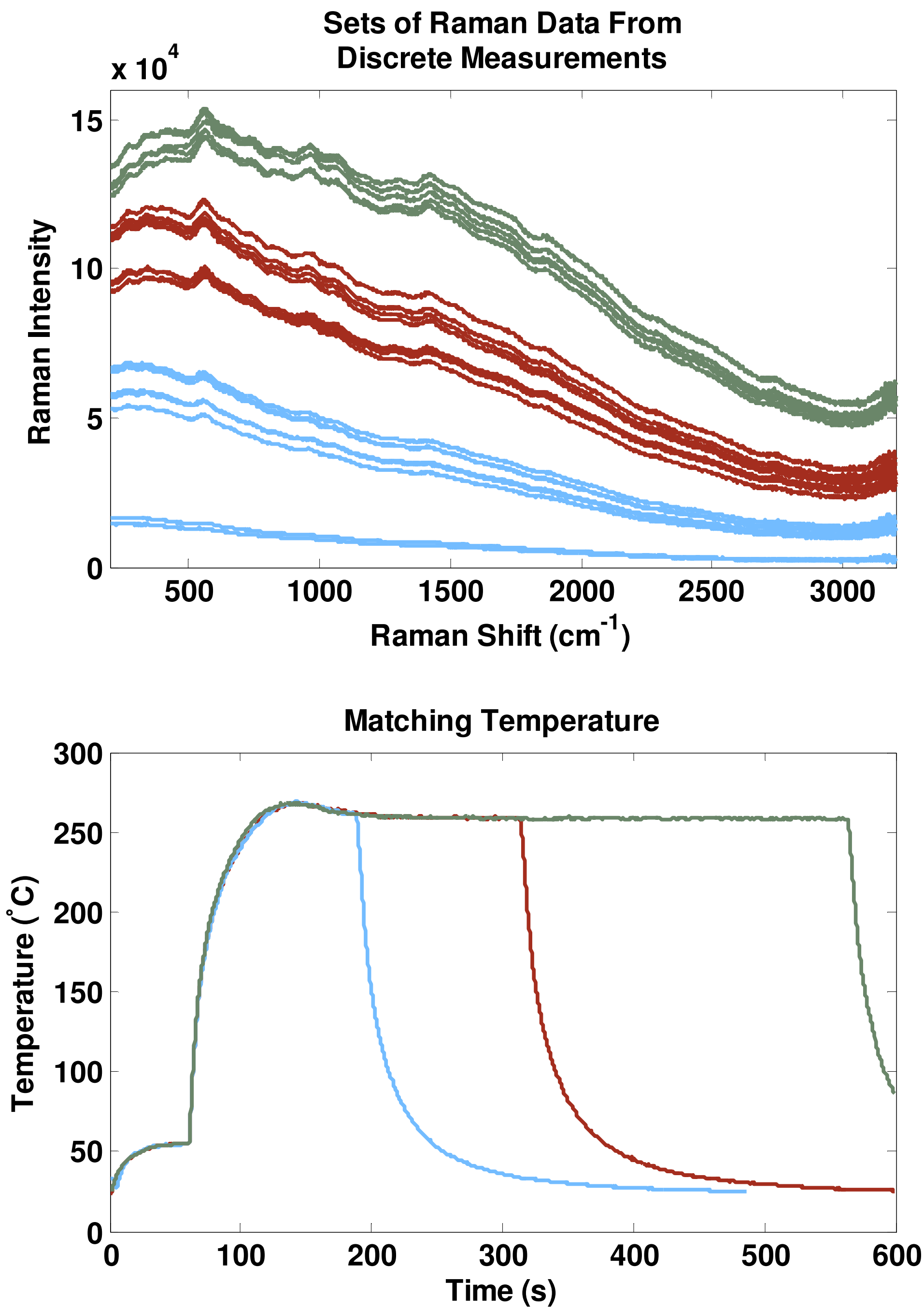


Figure 66. Raw Raman measurement sets from three of the discretely roasted coffee. These were chosen for display as they show common characteristics across all the discrete sets.

6.3.2.1 Variation in the High Frequency Component of the Single Bean Raman Measurement

Is there any Raman scattering information in the measurement sets? Although there are some obvious macro-changes in the signal (increased overall amplitude and slight twisting), they are more indicative of a fluorescing behaviour then Raman. A test was done to see if there were any changes caused by roast progression that were separate from the overall change in amplitude. The approach was to separate the large-scale differences from the small-scale changes using high and low pass filtering.

Figure 67 (top) shows the mean values of the 240 second – 600 second (4 minutes – 10 minutes) single bean Raman measurements. The bottom section of Figure 67 shows the same data over the same window after 5 repeated passes of running average 1-D low pass filter. This data was then normalised against its' mean to produce the result in Figure 68.

The data in Figure 68 can be examined to find no variations in the remaining middle frequency components. The remaining macro variations of the frequency components are dependent on the mean amplitude. This means that the overall amplitude is the most prudent measure of understanding the macro nature of these measurements.

Passing a low-pass 1D filter over the data removed the high frequency noise. The effect was dependant on the size of the filter and the number of repeat passes. The difference between the data with the high frequency removed and the original (non-modified) data, produced an array with only the high frequency component remaining. The extracted high frequency data can be seen in Figure 69.

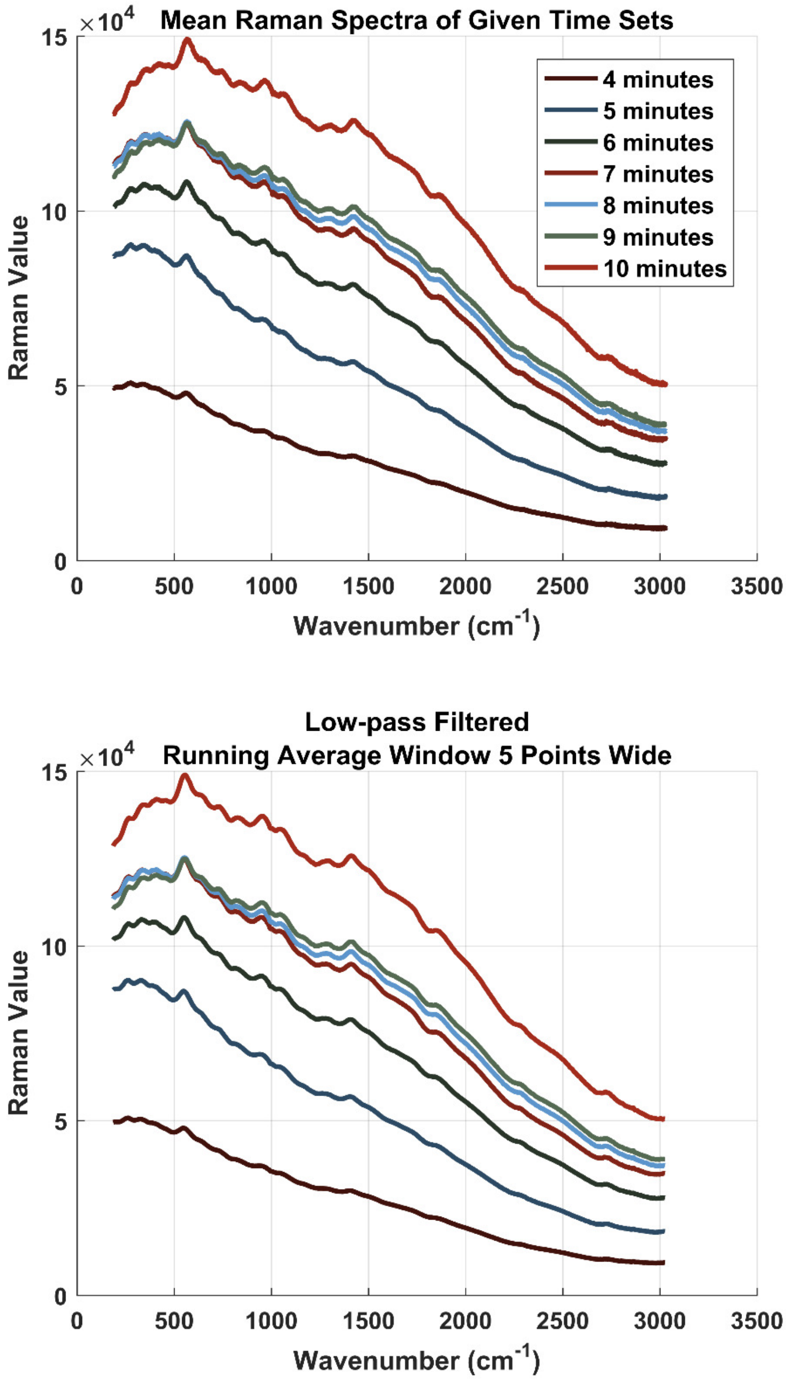


Figure 67. Means of single bean measurement (top) The data is displayed from a cropped window. Low pass filtered means of the same single bean measurements (bottom).

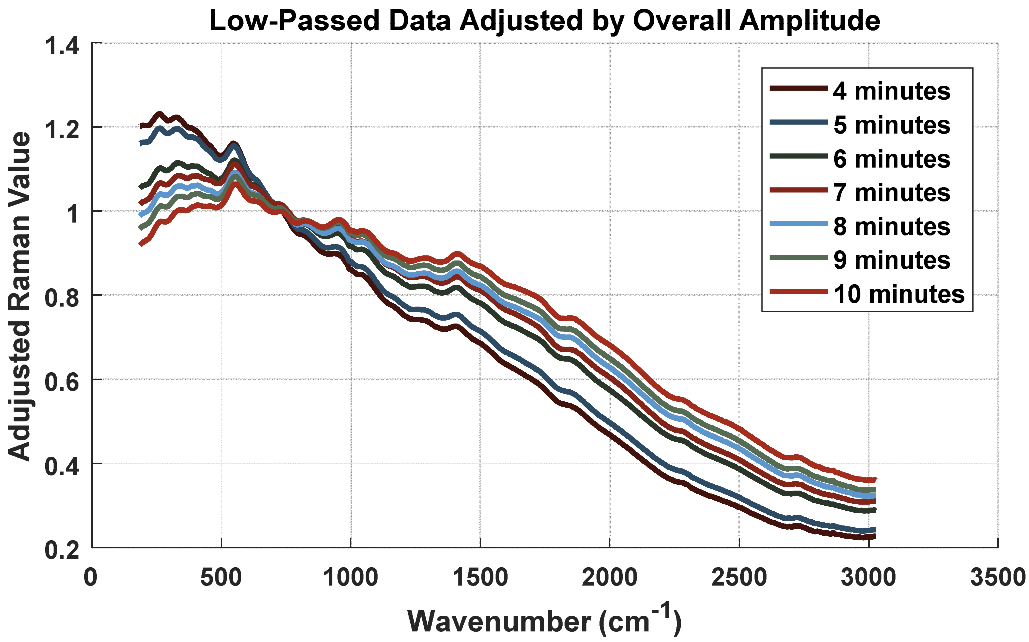


Figure 68. Normalised mean measurements.

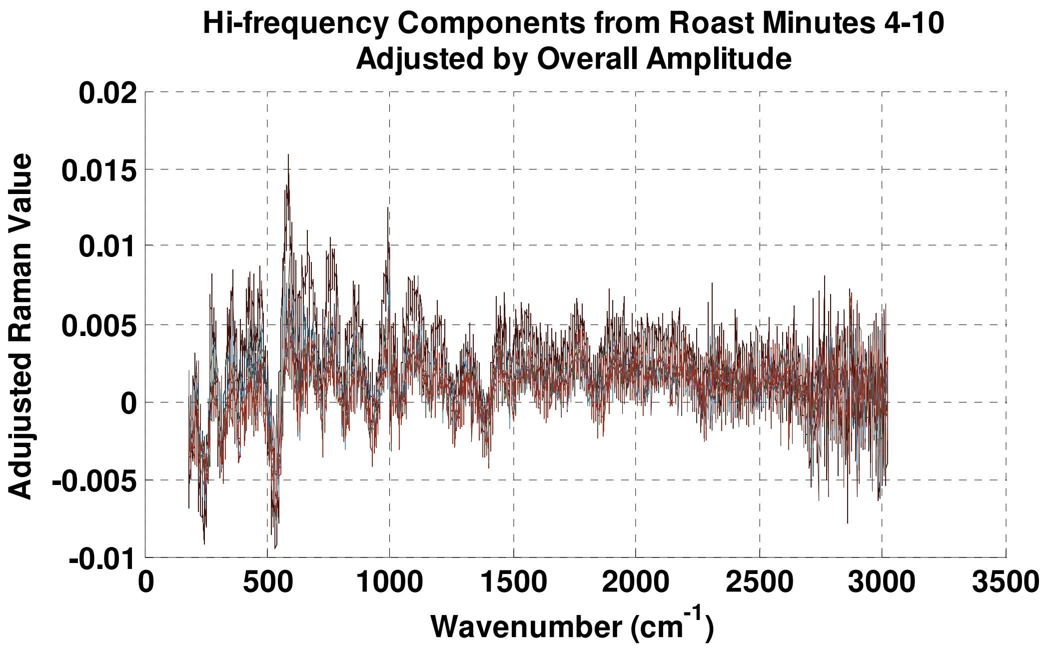


Figure 69. Normalised high frequency components of the data stacked on top of one another.

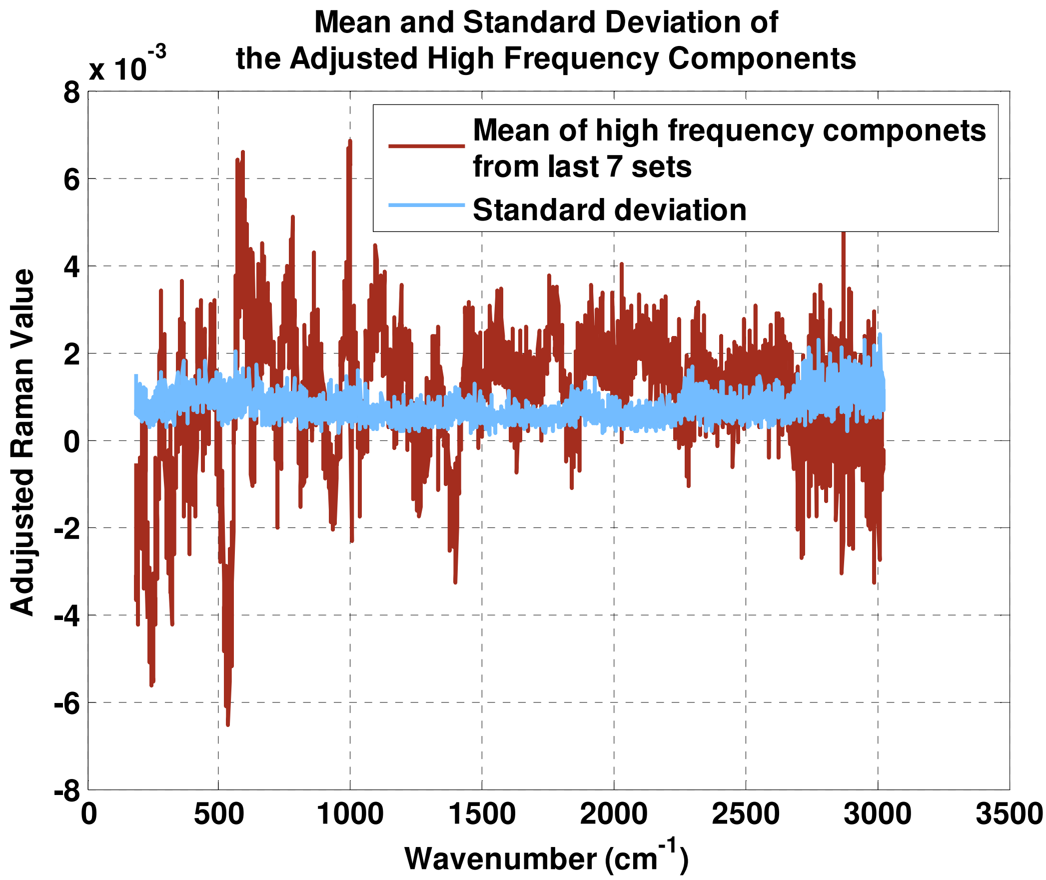


Figure 70. Mean of the high frequency noise measured by the Raman Spectrograph across various roasts.

The data in Figure 69 contains the high frequency noise obtained from the coffee roasted from 4 to 10 minutes. This is because the overall intensity of the measurements of green coffee, from 2 and 3 minutes, was significantly lower than the other displayed measurements. This meant that normalization caused the noise of the low time measurements to be amplified to a point where they were no longer useful for comparison. The mean of the comparable data was taken and is shown in Figure 70. This —when shown with the standard deviation— shows that there is no movement in the high-frequency peaks. This means that if there are any small signals that would come from Raman they are either not changing or not visible above the noise.

After processing, the conclusion was that there was no useful information stored in the frequency data. Therefore, what was being measured was changing levels of fluorescence. As the roast progresses the surface of the coffee becomes darker and fluoresces more. Therefore, a larger amplitude signal is measured during the later portions of the roast.

Why do beans of the same set give such a wide range of values? Focus, mostly. Having fixed laser power and exposure time should mean that measurements from the same bean should give a near identical answer. This is not what is seen. The major difference is the focus of the Raman spectrometer. This is clear in the coffee roasted to 200 seconds, Figure 66, where the data is clustered in two different sets.

It was unfortunate that the Raman data could not be extracted. However, the fluorescence does increase as roast progresses. The increasing fluorescence and its rate of change could be used as an indicator of roast progression. On top of that, the coffee examined in these tests was cold and had been left for a few days between roasting and testing. Although unlikely, it is possible that in-situ roast gives a result different from stale testing.

The major point to be considered in online testing was that the fluorescence was likely to saturate any Raman data. It would have been ideal if the fluorescence could have been reduced enough in-situ that Raman spectra became measurable. However, the Raman spectrometer could still be useful if it is possible to use fluorescence as a method of process control. For the fluorescence to be useful it needed to be consistent. To get consistent results, the way in which the laser was focused required careful consideration.

6.4 Fluid Bed Application

The plan for this experiment was to use the fluid bed roaster from the previous experiments. The roaster required little modification from previous experiments. It was set up with the glass roast chamber and could not have any extra insulation around the chamber. Beyond that, small changes were made to facilitate attaching the probe.

The most significant modification made to the coffee roaster was to address concerns about laser safety. The laser used by the Raman spectrometer was a class 3B infra-red laser. Lasers of this class possess a real risk in regards eye safety. To address these concerns a metal shroud was added to encase the roasting chamber and ideally any specular reflections from the laser. Additionally, anyone in the room while a test was being run were required to wear laser safety glasses.

Other changes included adding a claw to hold the probe steady during roasting, and adding a thermocouple to the end of the probe. This was to aid in protecting the probe from temperature damage. Figure 71 is a functional diagram of the coffee roaster modified to have the Raman probe attached.

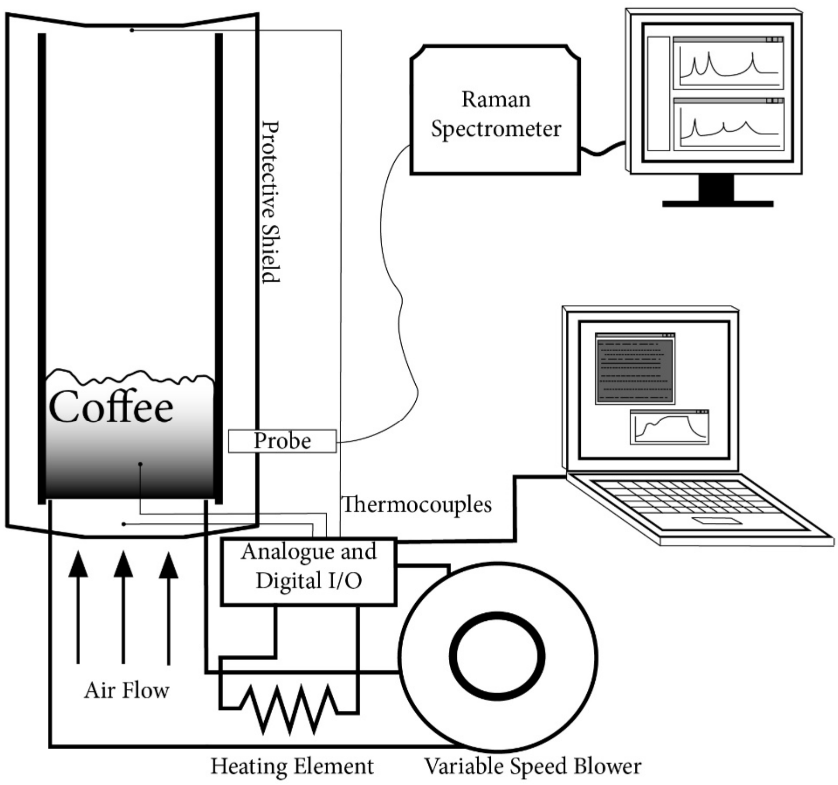


Figure 71. Functional diagram of coffee roaster connected to Raman probe.

6.4.1 Focusing the Probe

At this point, setting the focus of the probe becomes a major problem in producing consistent measurements. The probe had a 2.5cm focal distance. Setting the probe able to measure coffee was straightforward. The question then is how to get a consistent measurement when the subject is known to be moving in and out of focus? To ensure consistency all subsequent tests were done using a fixed capture/exposure length.

There are two possible ways of taking these measurements. Make the measurements on moving beans or on static beans. In the static case, the relative focus between the laser and coffee is fixed. Making static measurements on coffee will result in different levels of focus in each measurement. In most cases, it will likely fall in a similar distance however it is possible to get wildly different values (Figure 72). This means that relative fluorescence does not work with the static method.

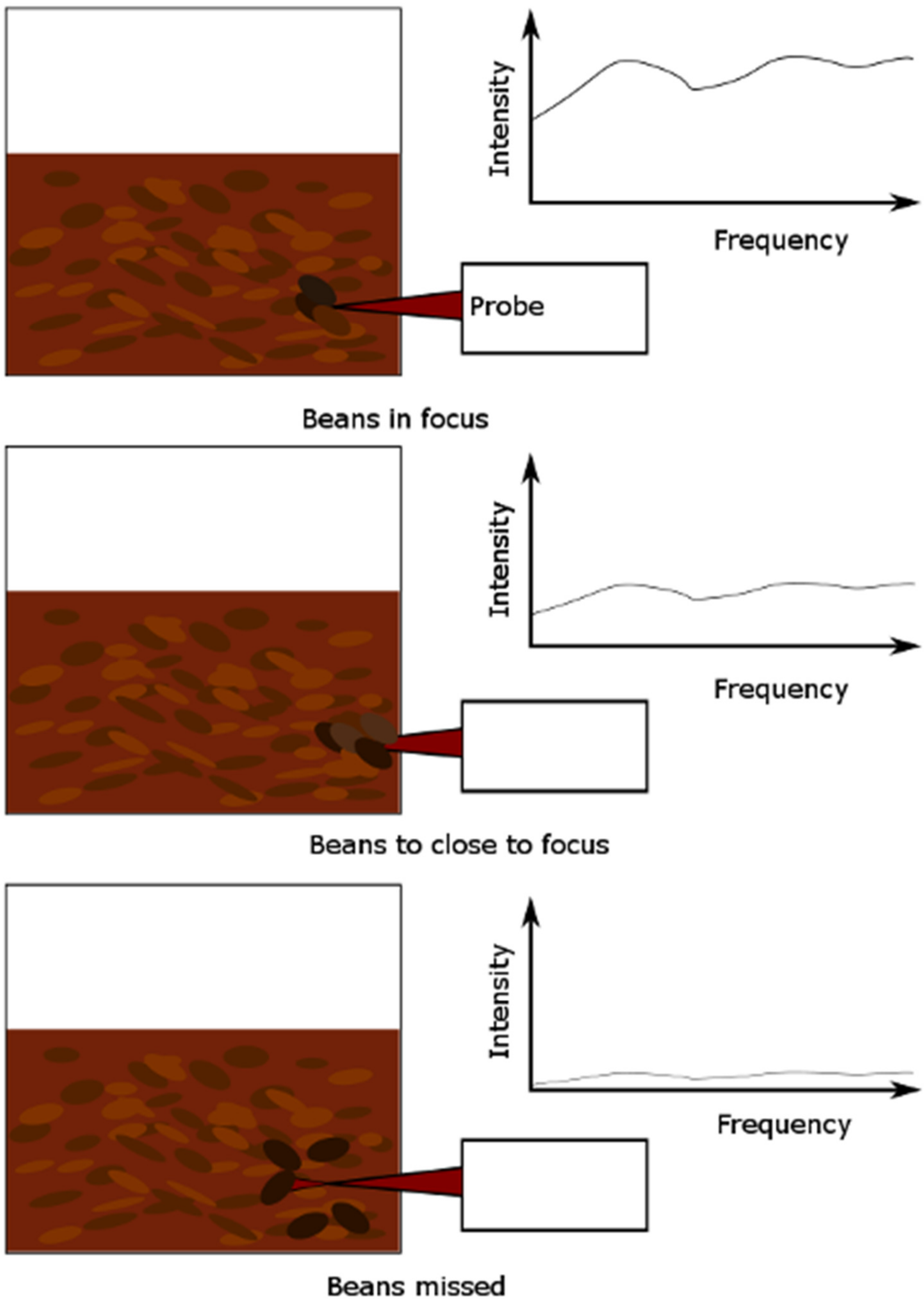


Figure 72. When using the fixed focal length probe in a changing environment, it is possible to get a different result without changing the probes position. The strongest signal will come when the target bean is in focus. Having the bean too close or too far will change the overall intensity.

The other method is measuring moving beans. The solution to the challenge of getting consistent measurements from moving beans, was to take a blurred capture.

Any changes in focus would average out, leaving the average florescence of the beans for that moment in the roast.

Specifically, when a CCD sensor captures light it behaves like an integrator and integrates the input light signal (Figure 73). This means that if the integration time (or capture length) is long enough, the result will be the average of the changing input. This will mean that the results are more consistent than in the static bean case.

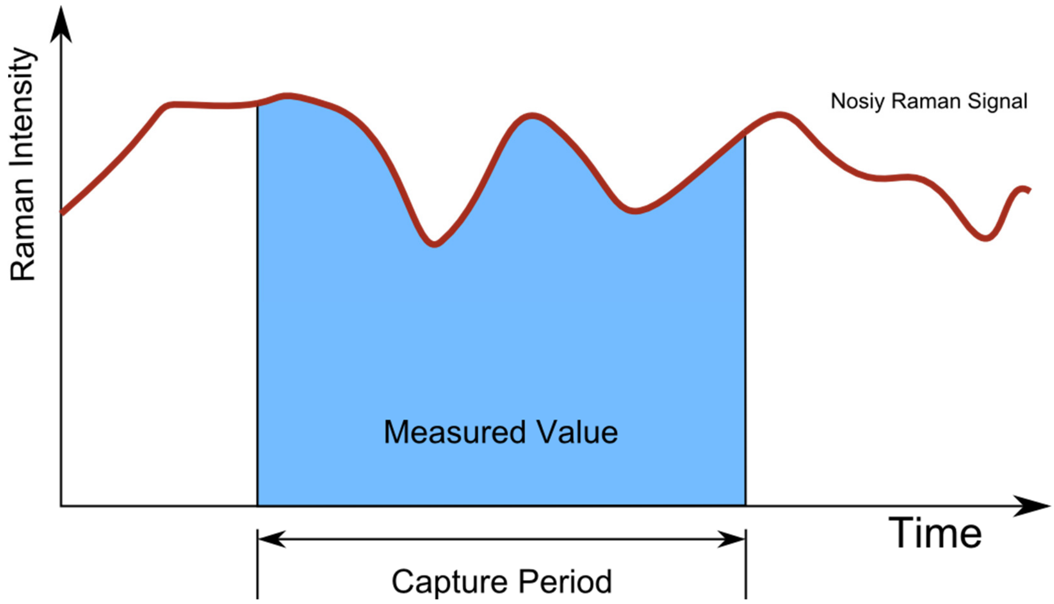


Figure 73. Illustration of Raman spectrometer's light sensor performing integration. Extending the capture period averages the changes in the environment.

6.4.2 Fluid Bed Results

To test the fluid bed measurement technique, the initial Raman measurements taken of the single beans roasted for different times were repeated in the fluid bed (Figure 74). For the most part, the beans returned similar signals to the ones produced in the single bean case, however they were all strangely distorted in a similar fashion. This distortion and how it is dealt with is covered later in the chapter. Firstly, the question answer is, do the fluidised coffee beans produce more consistent measurements than multiple measurements of static beans?

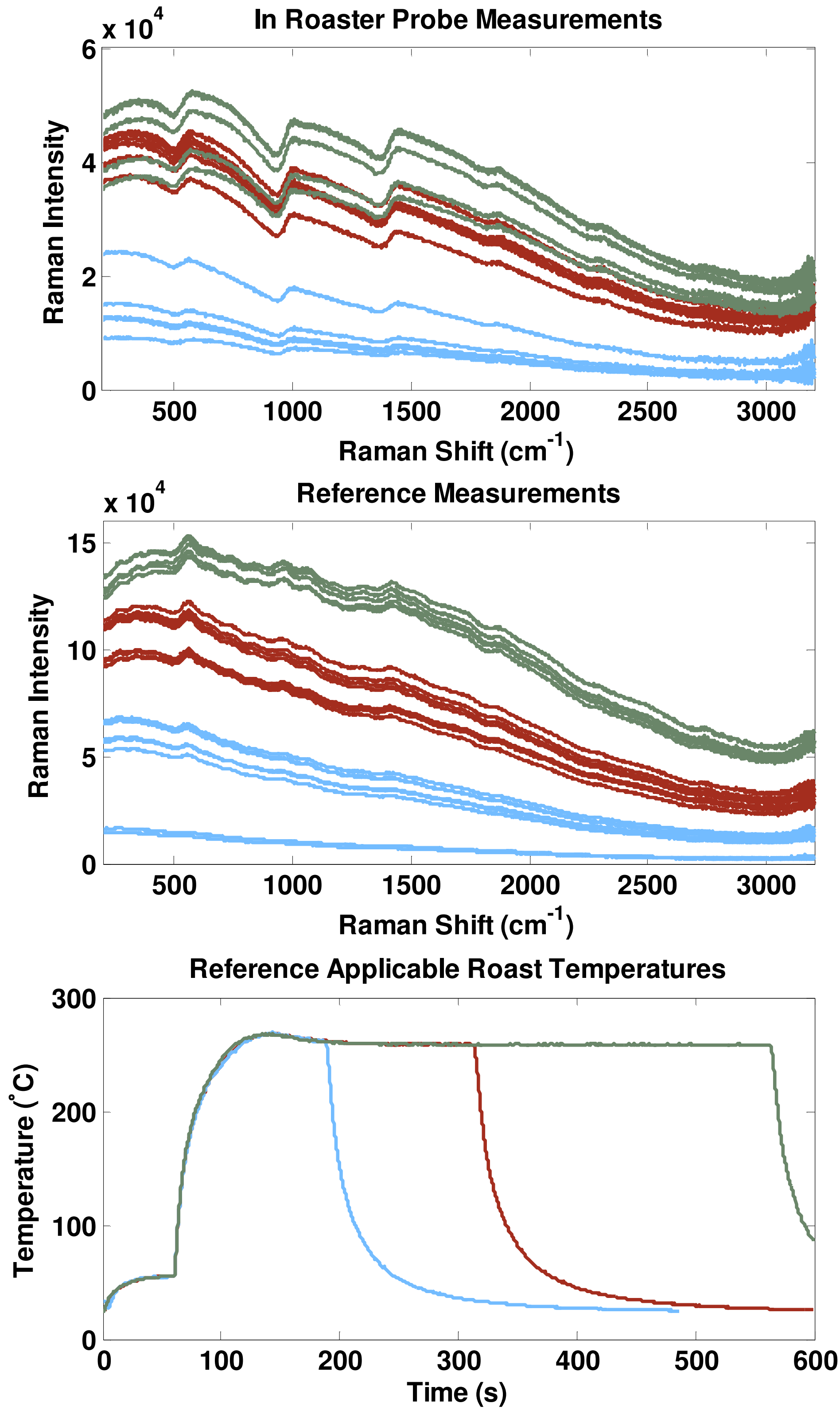


Figure 74. Measurements taken of the discretely roasted coffee (top) compared to the same coffee measured as single beans (middle). Applicable roasting temperatures are included (bottom).

6.4.2.1 Static measurements compared to fluid measurements

Using one of the pre-roasted coffee batches, a comparison could be made from the measurements taken by the two different methods; static and moving beans (Figure 75). What this shows is, the static measurements are occasionally close but have some very large outliers. The moving coffee on the other hand does not suffer from these outliers and is more constant. The observed behaviour agreed with expectation.

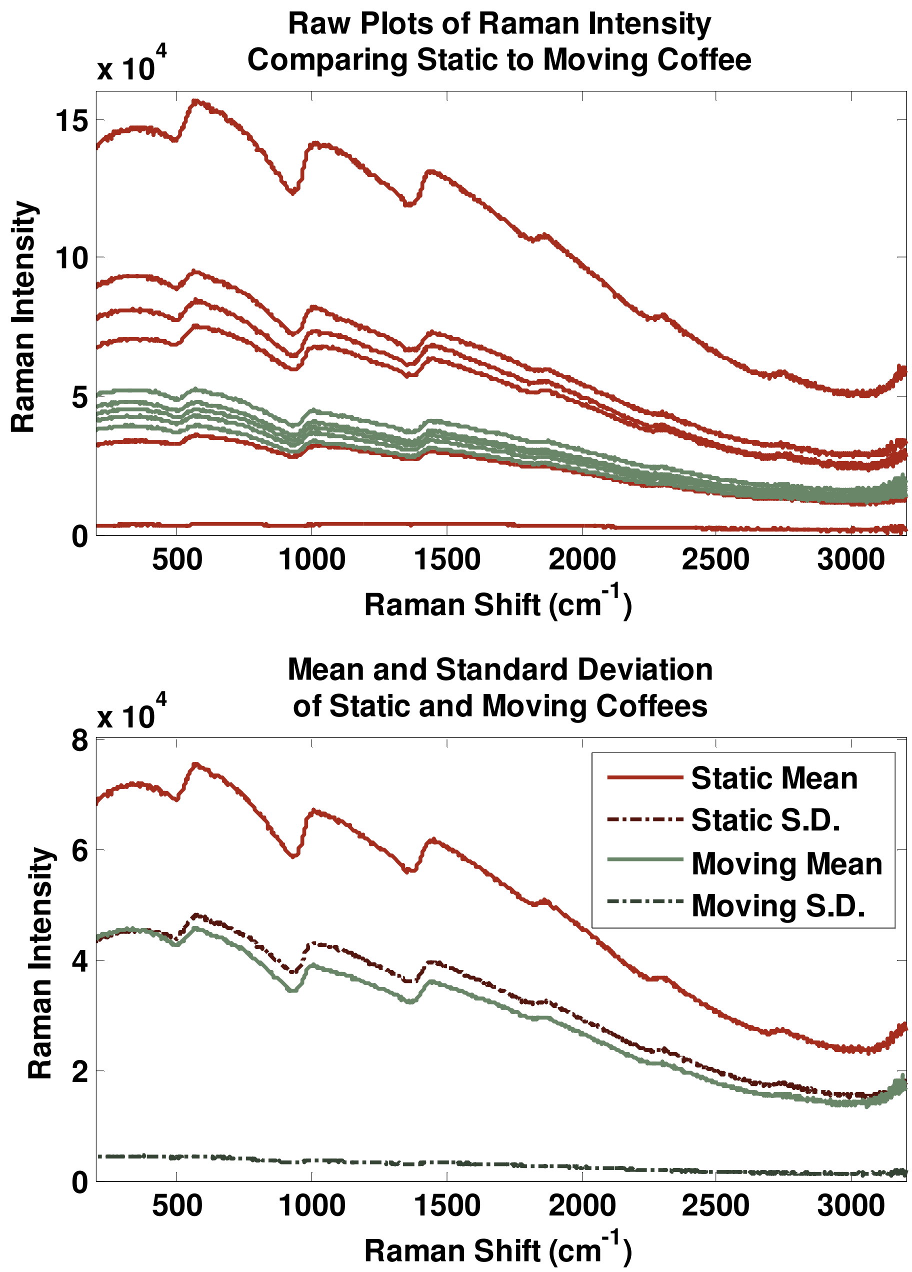


Figure 75. Comparison of static probe measurement to coffee in motion. Raw data sets (top). Comparing the mean measurements and standard deviation of the two sets (bottom), it is seen that the moving beans have a reduced average value but a much lower standard deviation. This was what was expected to happen.

6.4.3 Removing the Distortion

The next step was to address the distortion that appeared in the probe measurements. This distortion was likely an artefact produced by the Raman's echelle spectroscopy method. Echelle spectroscopy is method of gaining extra resolution out of a spectrometer. It works by splitting the light into multiple parts. The newly split parts are shone on to their own section of the sensor. The individual parts strike the sensor in separate places, meaning that a wider resolution can be achieved with the same sized sensor. A distortion similar to what is visible with the 'probe' measurements on coffee are shown in M. Pelletier's paper "Raman Spectroscopy using an Echelle Spectrograph with CCD Detection" [95]. In Pelletier's case, the distortion was displayed in his white light calibration and occurred where the individual bands were combined into a single spectrum. In the case of the 'probe' measurement, it is likely that the returned signal from the coffee is much broader and larger in amplitude than the PerkinElmer RamanFlex 400 was designed for. This means that the inbuilt correction was not sufficient.

A post processing correction was designed to fix the distortion. The distortion was consistent across all measurements; changing in amplitude as the measurement changed in overall value. This was addressed by comparing measurements taken from the Raman probe with measurements taken from the same sample on the Raman's translation stage.

Ideally the measurements taken by the probe and on the stage, should be equal. However, because the experimental setup is different and variables like the laser focus could not be accounted for, a direct comparison was not possible. To make the two sets of measurements comparable, each set was divided by its average value. This made each set comparable in size (Figure 76). This relationship was then used to find the distortion.

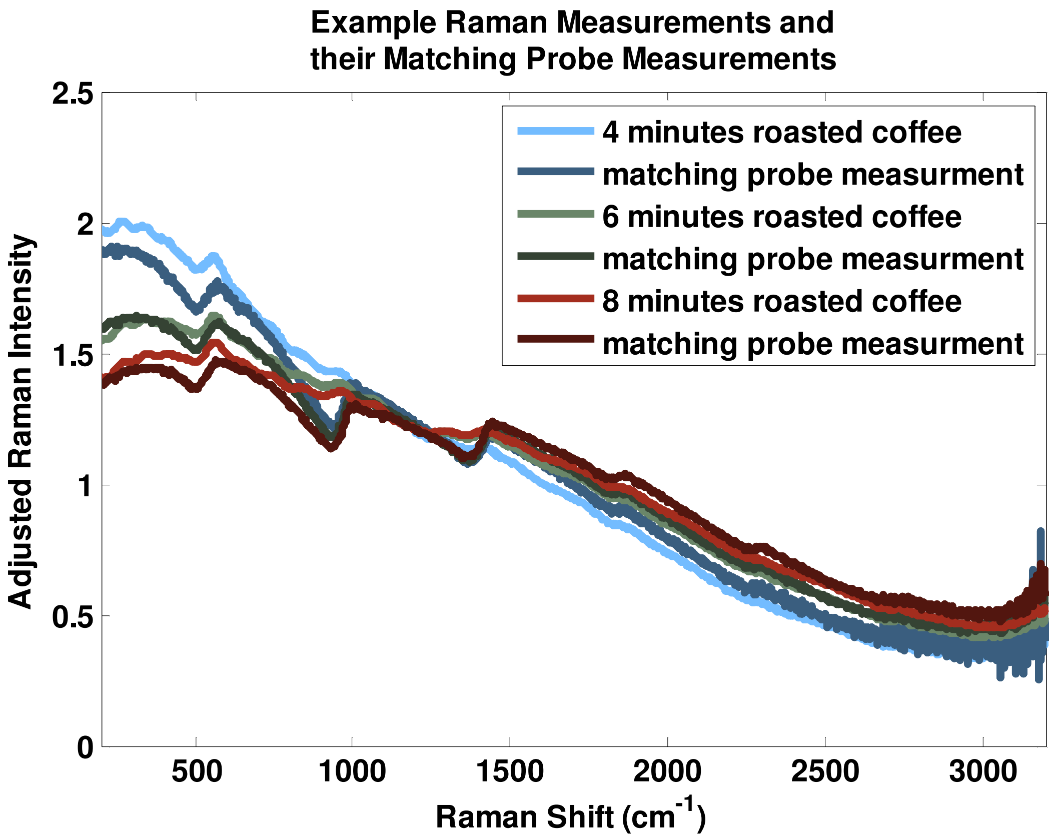


Figure 76. Dividing each measurement by its average causes the measurements to have the same average intensity so that they can be better compared. In this state, it is easier to observe the distortion produced in the probe measurements.

To find the distortion, the difference was taken between signals measured on the translation stage and with the probe (both adjusted to match). This produced a difference value that represented the distortion. The distortion was found to be consistent across all the samples (Figure 77). By using this value as a standard distortion, the process could be reversed and used to correct the distortion on all the probe measurements (Figure 78).

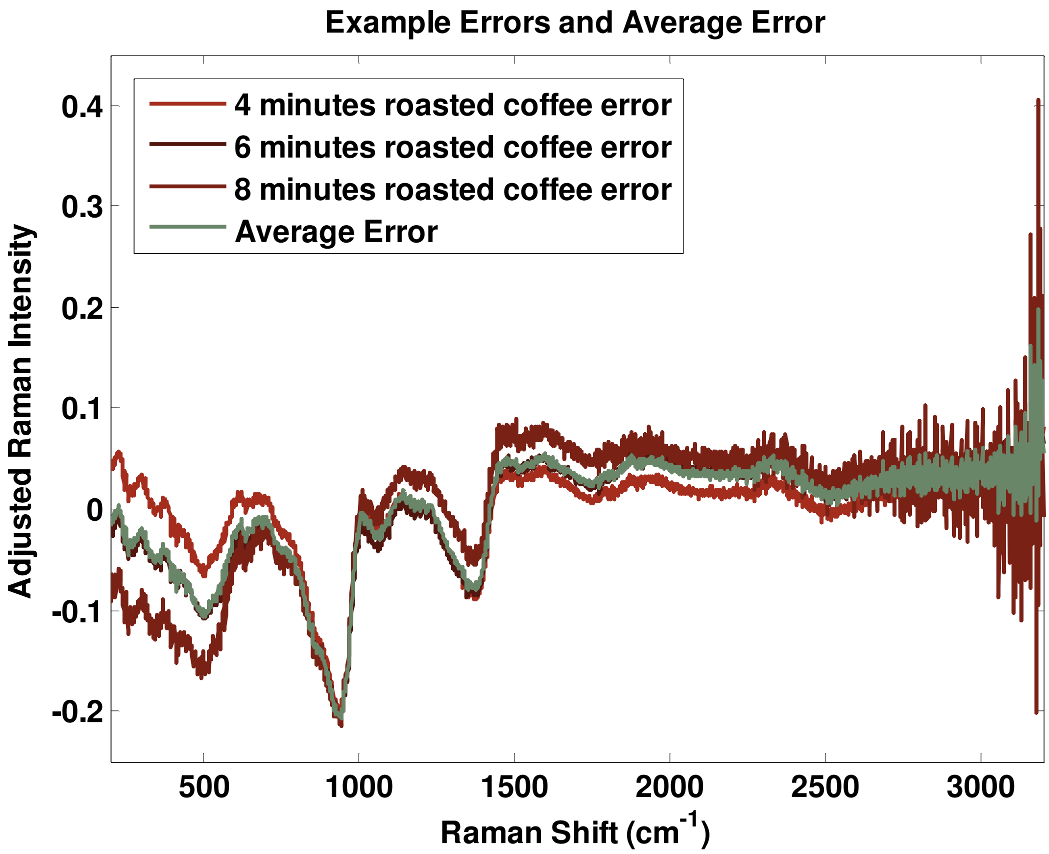


Figure 77. Taking the difference between the probe measured coffee and single bean measured coffee produced an error. This error was consistent over the different levels of coffee roast. This allowed for the calculation of the average error that was applied to correct future measurement.

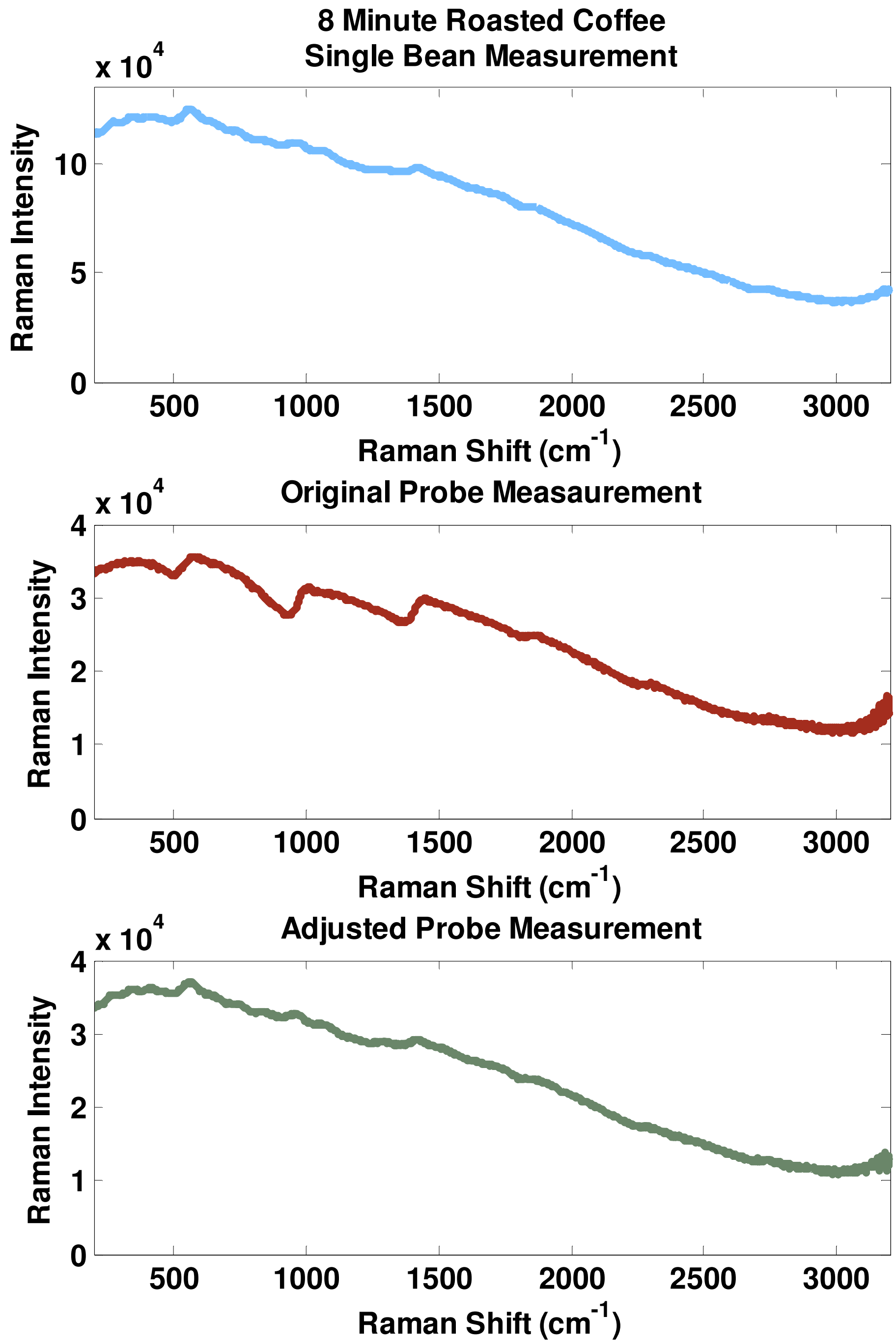


Figure 78. Single bean measurement of coffee roasted for 8 minutes (top). The same coffee measured using the Raman probe (middle). The same probe measurement adjusted using the average error calculated earlier.

This method removed the distortion to an acceptable degree. It corrected the data irrespective of the signal's size. A more complex model may have been able to correct the distortion; however, this method was straightforward and produced viable correction. This correction method could correct the results from the live roasting test.

6.4.4 Online Roasting Measurements

For the online roasting tests, a step roast profile was used (Figure 79). Online measurements produced the series of measurements seen in Figure 80. The distortion corrected measurements are shown in Figure 81.

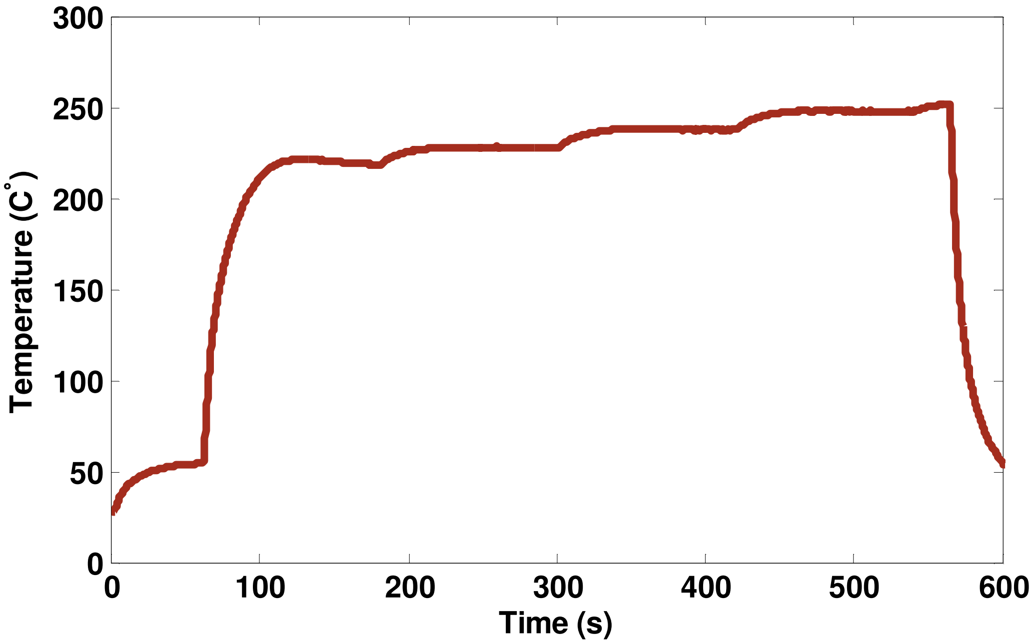


Figure 79. Step temperature profile used in Raman online roasts.

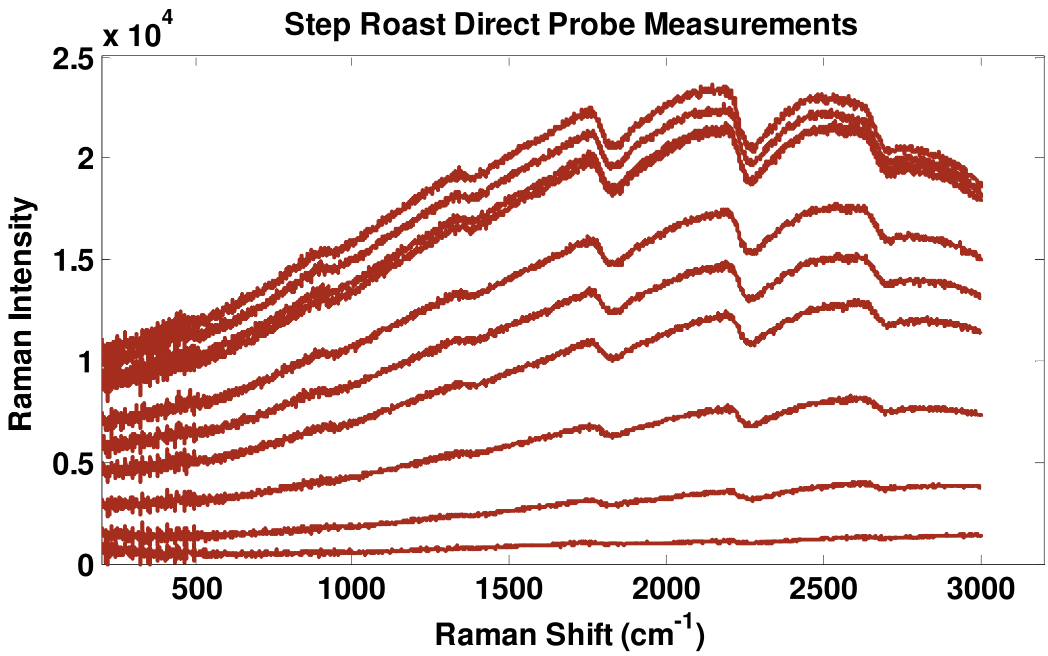


Figure 80. Raw Raman probe measurements taken of a ten-minute step roasted coffee roast.

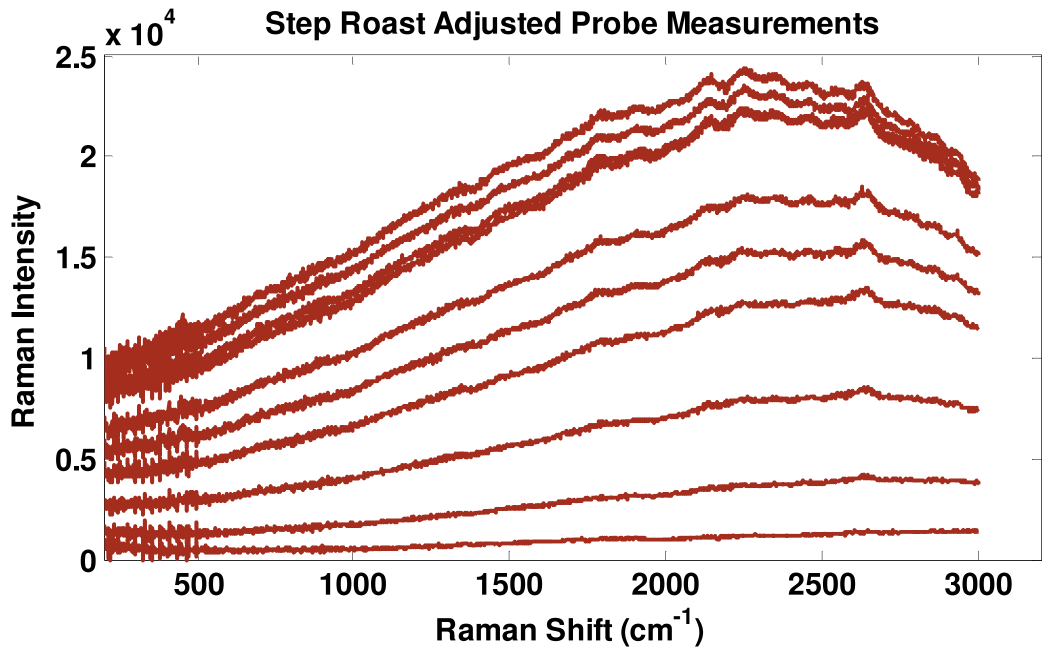


Figure 81. Same data from the figure above with probe error adjusted.

6.4.4.1 Results Analysis

As with the offline measurements the online roasted measurements did not contain any Raman data. The overall fluorescence did increase in a manner like what was expected from the earlier tests. This is plotted in Figure 82. The overall fluorescence didn't change much in the initial stages while the beans were heating. As the roast gets underway the fluorescence starts to increase. The increase remains relatively steady until near the end of the roast where it levels off.

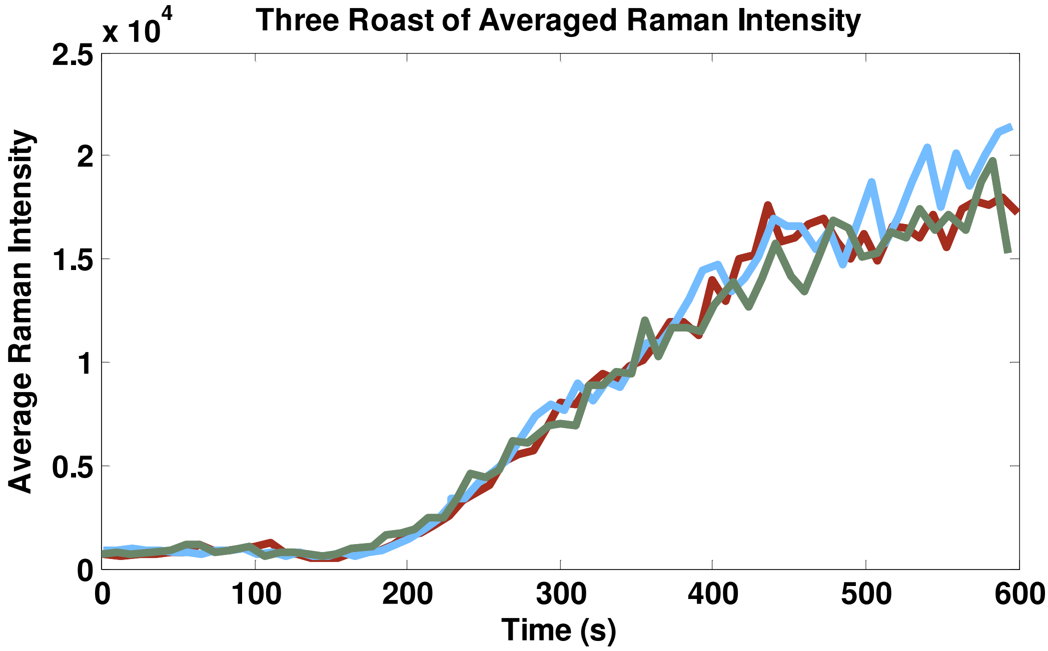


Figure 82. The increase in average Raman intensity, as the roast progresses

An average measurement can be refined by placing the data from all the roasts in a single array and then filtering that array. Further time domain filtering produces the plot in Figure 83. This tidies up the result and gives a better indication of the intensities change with roasting. Figure 83 also includes the approximate time that first and second crack were expected to occur.

In the early section of the roast the bean did not change much and very little change in the Raman signal is observed. In the early to middle section of the roast, the colour of the bean started to yellow and darken, this lead to an overall increase in Raman intensity. The darkening and increase in Raman continued for the rest of the roast. The rate of increase of Raman intensity noticeably decreased toward the end of the roast; this was put down to the coffee colour becoming more stable after the major coffee roasting reactions have been completed.

The Raman intensity also became less stable toward the end of the roast. This was likely due to the lighter density coffee moving more quickly. However, this meant that finding a constant transient was all but impossible. The point where the decreased stability occurred was around the same time as second crack. If the measurement procedure was tuned, this technique could be used to monitor roast progression. But could not be used to detect the ideal end of roast time.

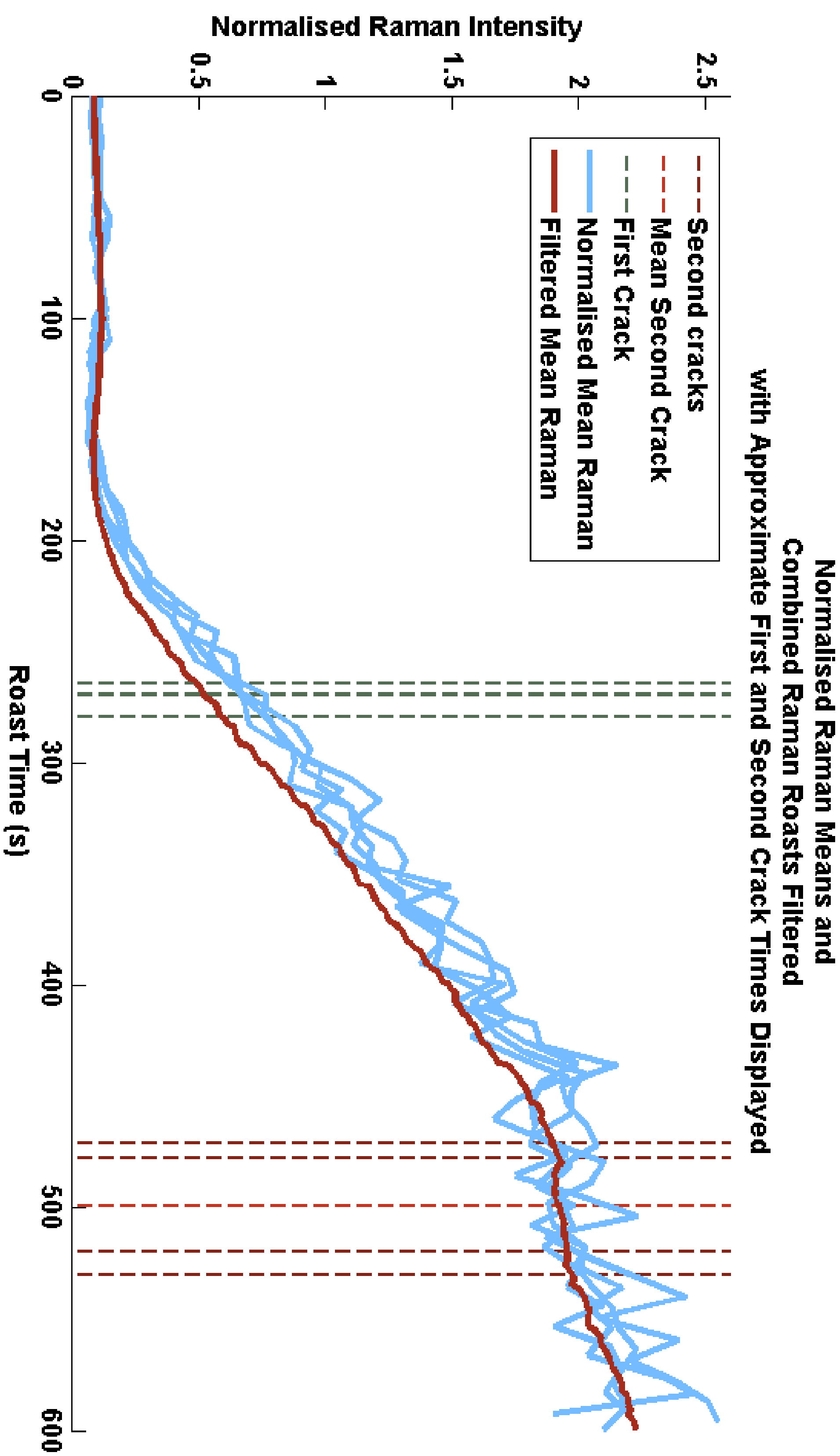


Figure 83. Scaled filtered Raman averages plotted with approximate “Crack” waypoints

6.5 Application of Thermal Model to Raman Data

The same glass chamber that was used in the thermal testing was used in the Raman tests. This meant that the thermal model could be applied to these tests. This application worked better than the application to the stainless-steel chamber. The comparison between the model and the Raman data can be seen in Figure 84. This figure shows a comparison between the increasing overall Raman intensity and the modelled moisture content as the roast progresses.

Figure 84 illustrates what has been seen with most of the measurements taken up until this point which is; there is a strong obvious change in the measured parameters; these changes are not obviously independent; and there is no rapid measurable consistent transient change in the coffee that could be used as a previously unknown waypoint.

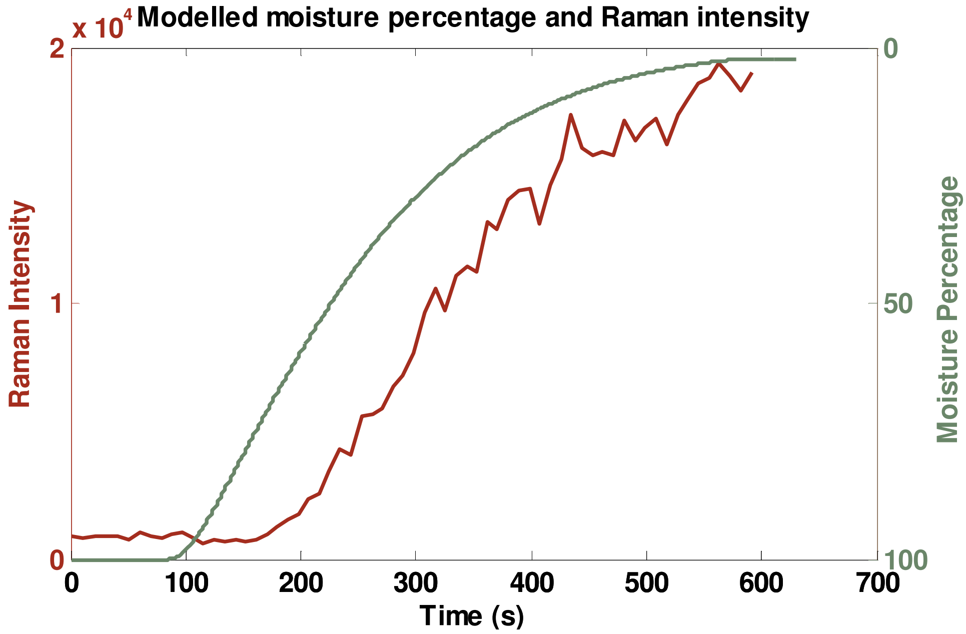


Figure 84. Modelled moisture content compared to the increased Raman intensity.

6.6 Conclusions

This chapter covered the use of a Raman spectrometer for the online monitoring of roasting coffee. This was possible by this by fitting an external probe from a Raman Spectrometer onto the glass chambered coffee roaster. Before taking online measurements, a matching set of baseline Raman measurements were taken.

The first Raman measurements were on a series of coffees roasted to different levels in a controlled environment. This allowed for the observation of how the progressing roast changed the measurements. These measurements were used to determine that any Raman data was being saturated by fluorescence. However, the fluorescence's overall amplitude increased consistently with roast progression. This meant that even though Raman spectra were undetectable, in the online roast, fluorescence could be used in this setup as a measure of roast progression.

The problem with the plan to use fluorescence as a measure of roast progression was the amplitude being, both, a function of roast progression and the focus of the Raman probe. Meaning that changing the focus — or in the case of the fixed focus probe, moving it — changed the overall amplitude. This needed to be addressed when moving into online testing.

In the initial Raman probe measurement, the goal was to replicate the results measured in the controlled environment. Also, it was to test the theory that by having the beans moving in the fluid bed during Raman capture it would produce a consistent measurement without knowing the exact focus of the Raman probe. The probe measurements produced results like the ones measured offline but they contained an unusual distortion.

The hypothesis that moving coffee would produce a more consistent measurement than static coffee was tested by comparing the Raman spectra taken on a single set of roasted coffee beans in both conditions. The coffee measured while static returned consistent results but changed wildly after moving in the fluid bed. The measurements of fluidised coffee returned a much closer set of measurements, showing the theory was correct.

There was a notable distortion that was introduced when using the external probe. This was removed by comparing the measurements taken on the single beans in the controlled environment with the measurements taken on the same coffee in the fluid bed. The comparison allowed the extraction the common error in the different measurements. The error was subtracted from future measurements, removing the distortion.

With the focus issue resolved and the distortion removed, the data from online coffee roasting could be analysed. The results, expectedly, did not show any discernible peaks caused by Raman scattering but did show an increase in overall fluorescence intensity with roast progression. The fluorescence's intensity showed a consistent pattern as the roast progresses. In the end however, using the fluorescence, there is no detectable pre-second crack transient that could be used in the detection of second crack.

This method could be used as part of a system of other online sensors to determine roast progression. Also, the method of measuring large particles in a fluid bed may have uses for other applications. This method did not achieve our desired goal and it would likely be easier to achieve this result using a colour sensing method as described by Hernández et al [60].

7 Conclusions

Coffee roasting has long been considered an art, and this work has shown that there is good reason for this. Sensitive measurements of phenomena measured in real time on a purpose-built fluidised-bed roaster were used to uncover the science underlying the “Art” that expert coffee roasters are implementing. All the tested sensor methods confirmed that there are no specific or perceptible changes exactly associated with roasting beans reaching some objective, ideal point that delivers maximised taste quality.

In the case of the thermal analysis, the concept of "bean load” permitted detection of thermal events in the progress of the roast—calorimetry in real time— including measurement of energy lost to evaporation. Measurements showed that there are no events that could be detected by calorimetry in the region where the roast is known to pass the ideal endpoint. These measurements were reflected in a numerical model of the roasting system. Agreement between measured and modelled data lent further confidence to the negative finding.

The microwave measurements allowed, by the use of a microwave resonating roasting chamber, the online changing permittivity measurement of roasting coffee. The measurement showed a smooth progression in the change in the cavity’s resonance. This showed there is not event present that could be used to identify an ideal end of roast. The smooth progression produced by this measurement matches that found in the thermal measurement case further reinforcing the negative result.

Although the microwave measurement techniques developed in this thesis did not find the desired transient, the technique created, opens opportunities for other types of qualitative microwave aquametry applications. The qualitative technique offers a level of flexibility in microwave aquametry applications not seen in literature. Present techniques are quantitative, and only function correctly when the system is tightly controlled. A qualitative technique could be used where the application dynamics preclude a favourable microwave aquametry setup. Such applications would include restrictions such as unknown or changing resonant chamber size; or changing sample position, or temperature. The image based technique allows for the relatively simple deployment of a previously difficult microwave aquametric system.

Use of a Raman spectrometer produced a method of measuring the increase in the coffees surface fluorescence during roasting. As with the previous two measurement methods the result was a smooth progression throughout the roast. Meaning that the measurements showed no events toward the end of roast that could be used as a method of detecting ideal end of roast. The similar results from all three measurement methods leads to the conclusion that they are all measuring similar or dependant phenomena.

7.1 Conclusions for the Master Roaster

The results of this thesis show that all the easily observable phenomena are essentially flat, this leaves the question open “How are master roasters making end of roast decisions?”. This leads to the conclusion that the so-called roasting experts are not using a perceivable waypoint to make decisions on roast completion. Nevertheless, the data and experience established in this work points to two possible scientific mechanisms by which a roasting expert may be locating their endpoint. The first is interpolation.

First crack and second crack are two obvious waypoints in the roasting process. Second crack is generally accepted as indication that the roast has gone too far. The author and his supervisor observed many roasts in person and through recorded video. What is less frequently observed is a master roaster making a mistake. When switching from beans of one provenance and age (“origin”) the expert roaster will often ruin a roast, or if not ruin it, then produce a roast far from ideal. Fastidious roasters will throw the batch out. In effect, the roaster must calibrate themselves with each change in origin. The author speculates that the roaster has found through trial and error that the ideal endpoint occurs a given time after an obvious waypoint, say first crack. Provided the roaster is careful to repeat the procedure exactly from roast to roast, the ideal point will always occur at the same time. That time was found by interpolating between first crack and second crack.

This mechanism is consistent with the care taken in machine setup and weighing of the incoming batch. It is consistent with the periodic wastage from burnt batches. Interpolation does not require the sense of smell, valued by many amateur roasters but essentially unavailable to commercial roasters whose machines must vent or even scrub their exhaust for health and safety reasons.

The second mechanisms by which master rosters can control end of roast is to use smell. This is a mechanism that has only been observed in use by amateur scale coffee roasters because of the unavailability to commercial users. Looking at the results from the SIFT-MS and Laser Ionization-MS [33], [34] it appears that the roasters who use smell as an endpoint detection are simply catching the beginnings of second crack.

Examining these two end of roast control mechanisms leads to an idea of "roast spread" Figure 85. All the coffee beans in a roast will have varying roast degree, the average degree of roast will be spread out in a bell curve. The standard deviation of this bell curve is the "roast spread". The smaller the roast spread the more uniform the roast. Considering the roaster who uses smell as the primary method of roast control. It may well be that they wait until the beans are very near second crack, when the first pyrolytic reactions that form second crack start producing volatiles. These volatiles are what the roaster is hoping to smell as an end roast indicator. The level of these volatiles that the roaster is wanting to detect is very low. In this case having a slightly wider spread will ensure that the roaster catches most of the roast correctly. The human nose is very sensitive and is likely better than most simple volatile detection methods, however a technology like SIFT-MS could be a very useful addition to the field of coffee roasting.

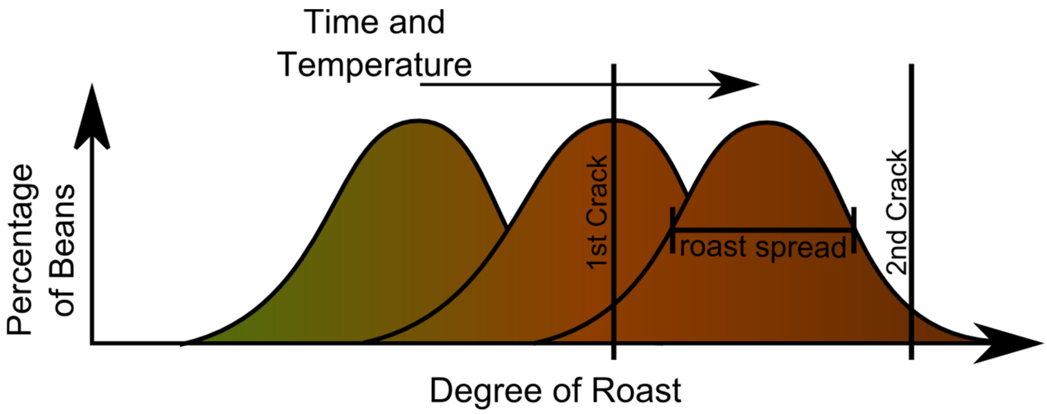


Figure 85 Illustration of "roast spread" as a roast progresses

From personal observation, there is more than one factor that affects roast spread. These include but are not limited to the origin of the beans and roasting technique Figure 86. This also may highlight the popularity of drum coffee roasters in commercial facilities. It is likely that the drum roaster produces a very consistent and (relative to a fluid bed) wide bean spread. This would therefore make it very useful to an expert predicting end of roast via extrapolation. A wider spread would also allow for a larger percentage of "good" coffee if some coffee is over roasted. Additionally, consistency would allow a roster to be more certain of the result.

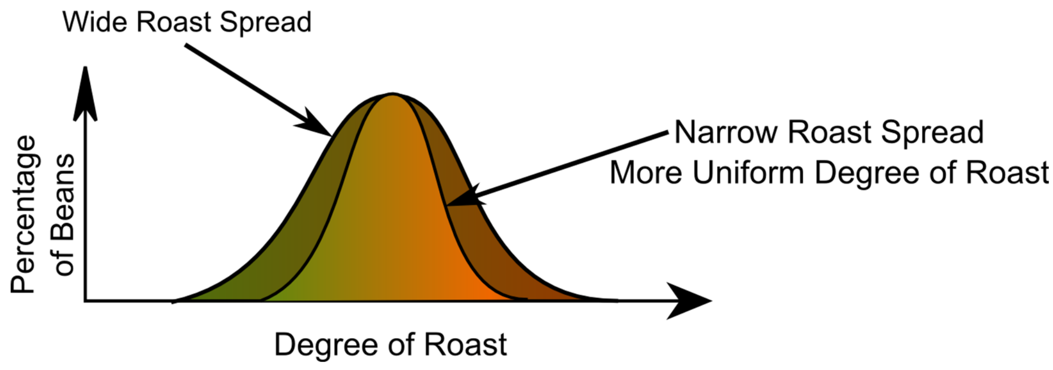


Figure 86 Comparison of two different "roast spreads"

Since the early coffee literature [5], [28] much progress has been made into the understanding of coffee and its roasting methods, this thesis adds to this knowledge. Whatever the outcome, it is clear that there are still many issues yet to be addressed.

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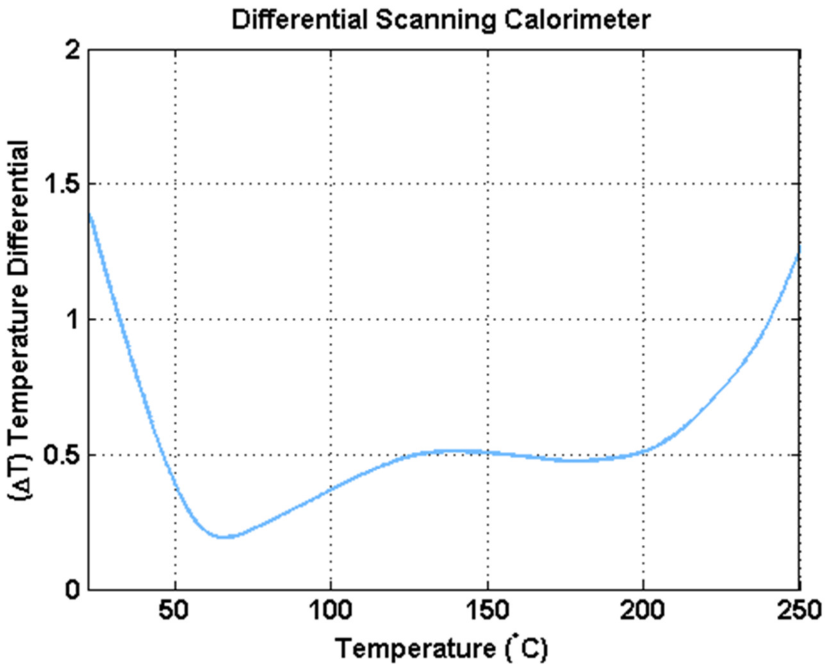
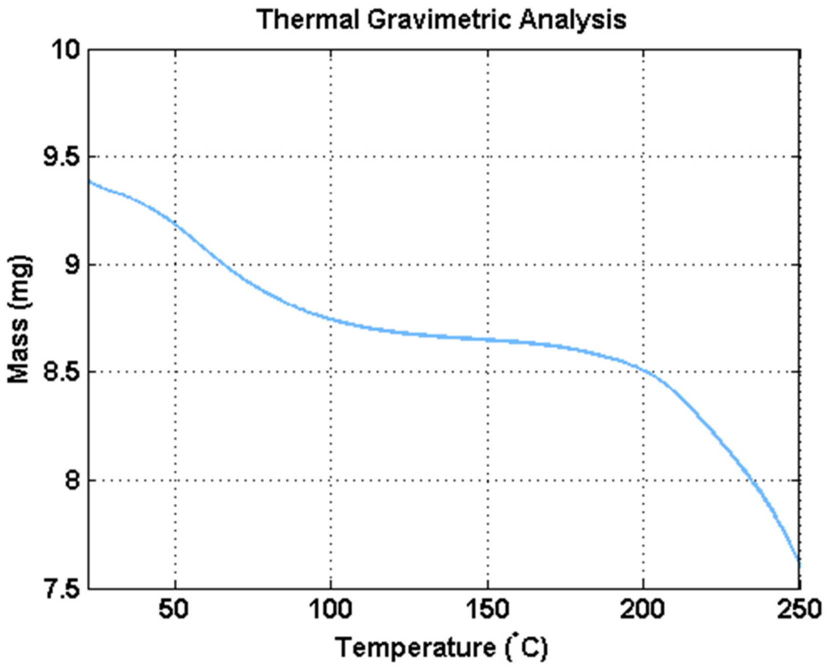
9 Appendix

9.1 Calorimetry Measurements on Ground Green Coffee





9.2 Stainless Steel Coffee Roasting Chamber

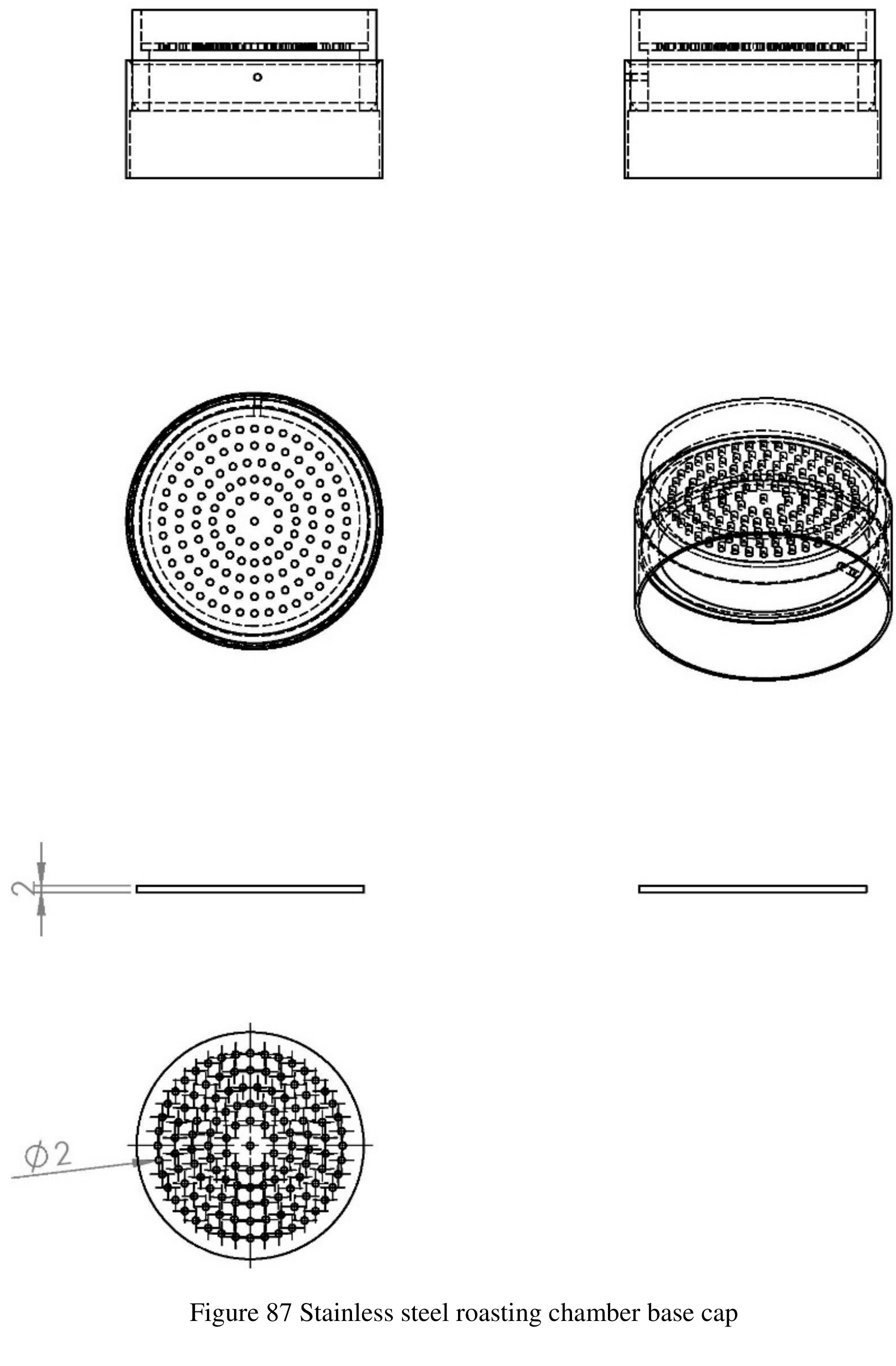


Figure 87 Stainless steel roasting chamber base cap

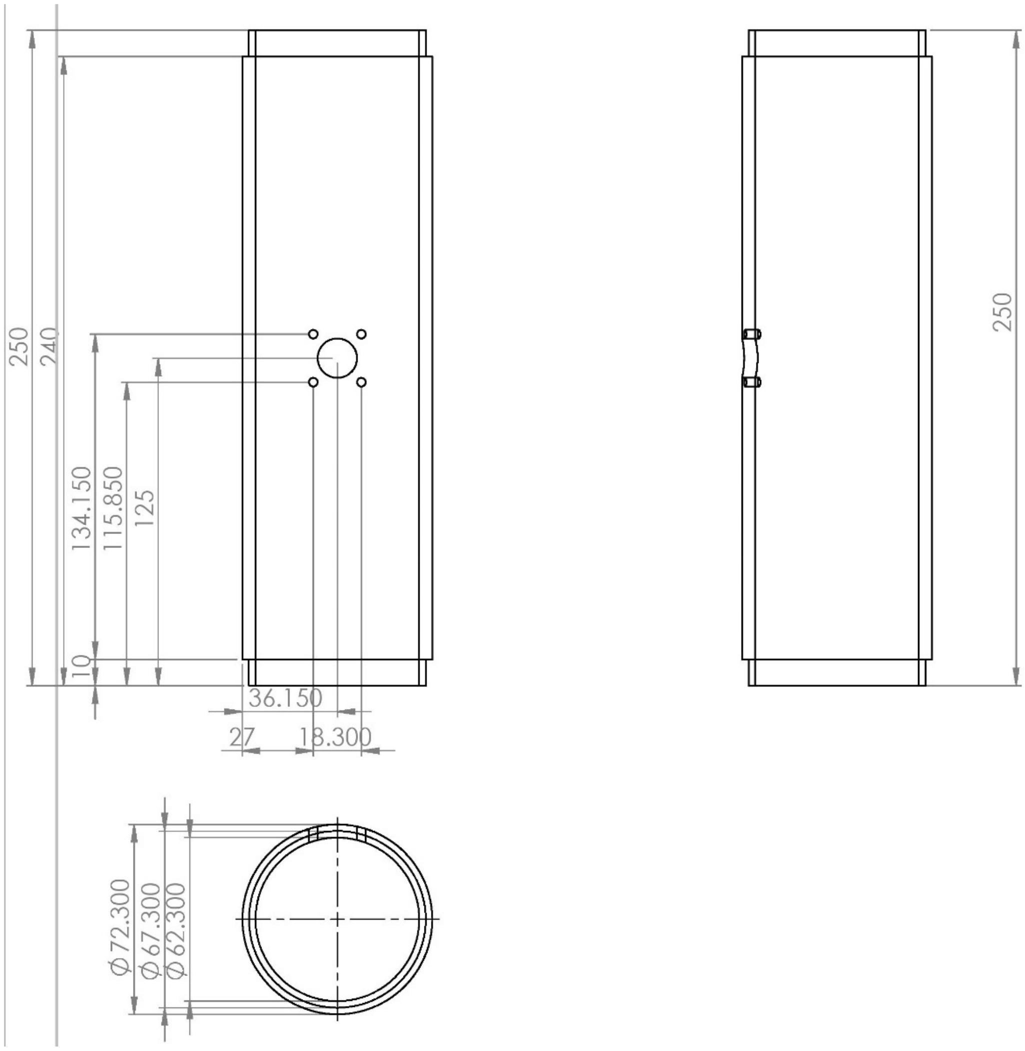


Figure 88 Stainless steel roast chamber main body

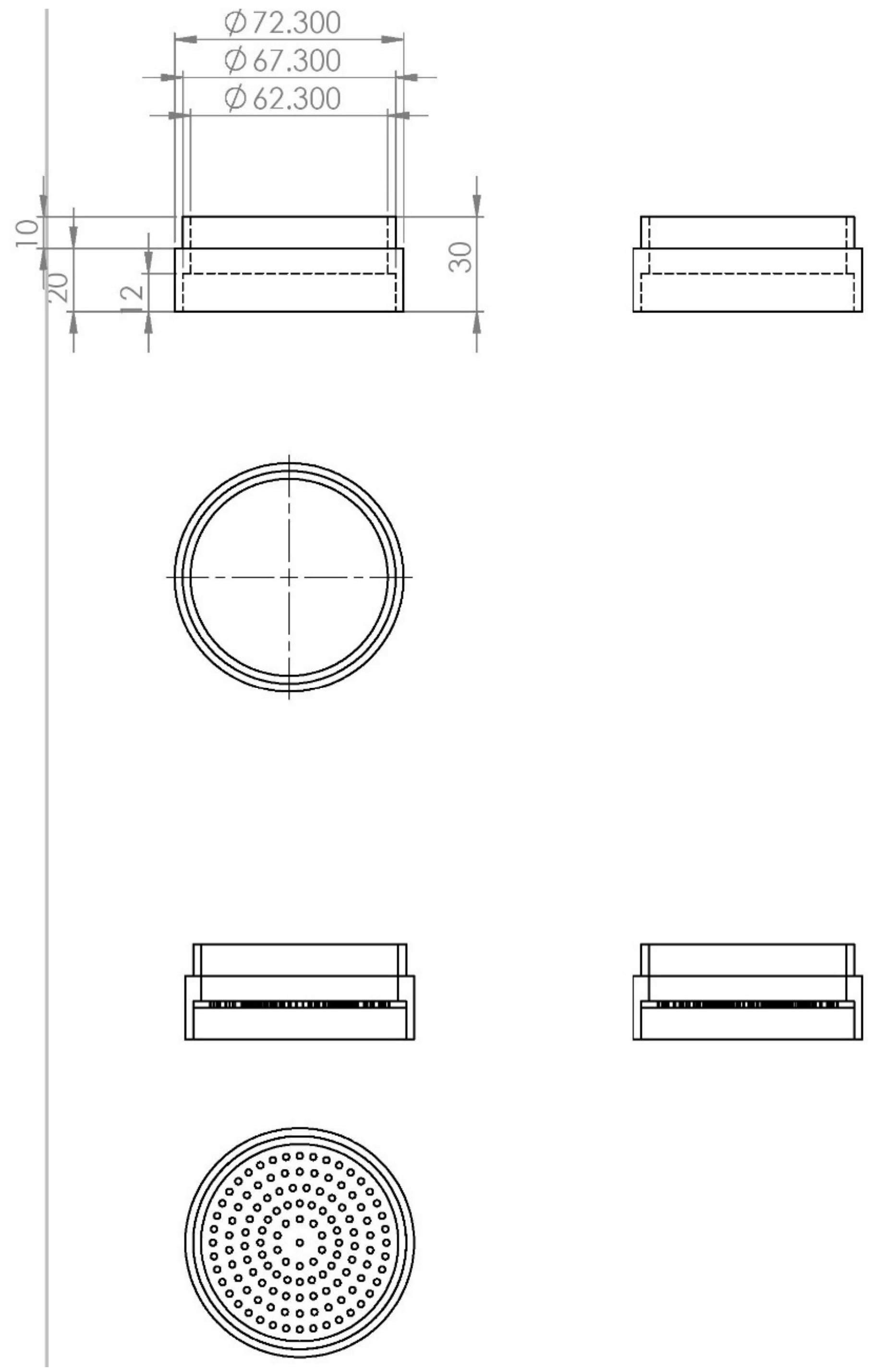


Figure 89. Stainless steel roast chamber top cap

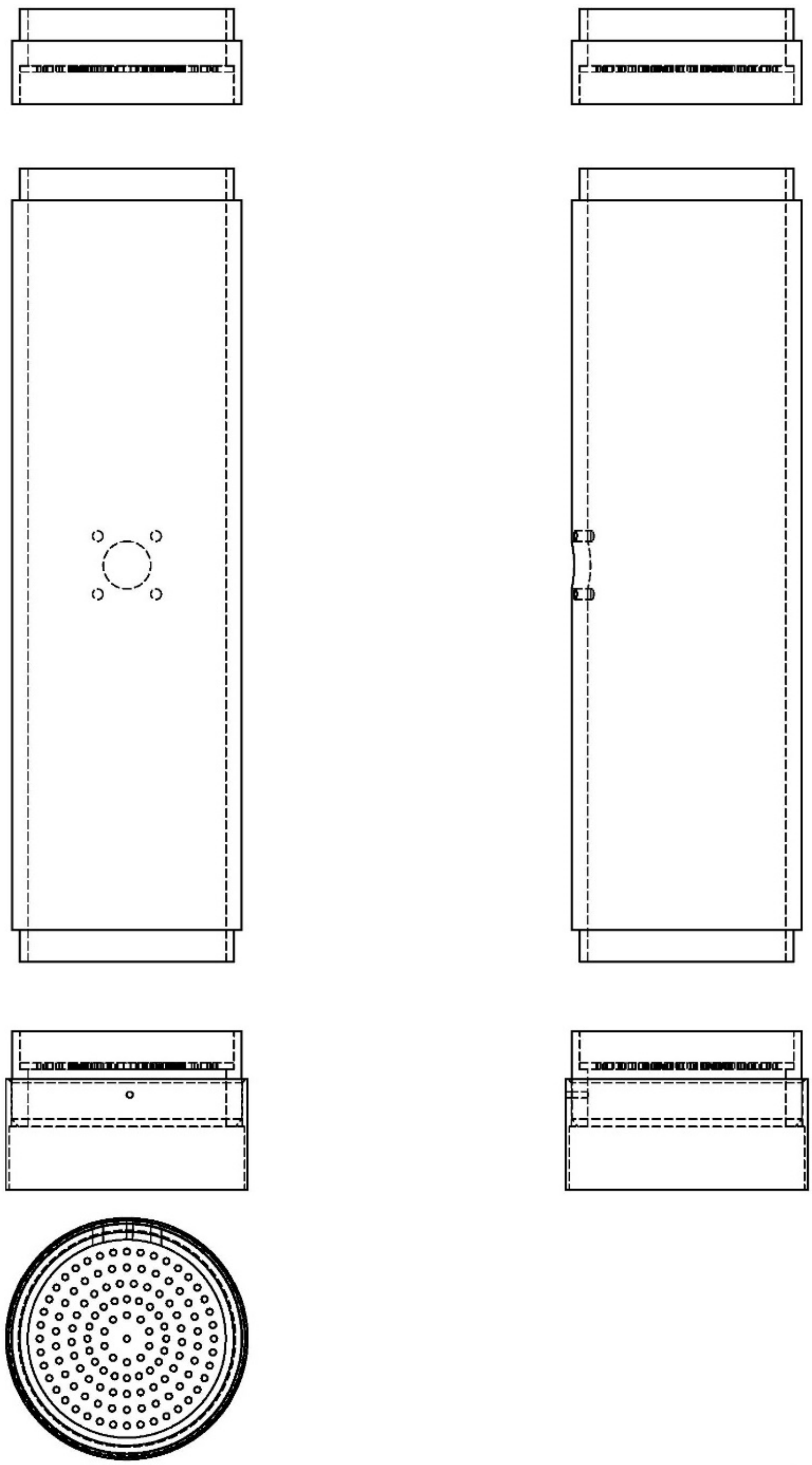


Figure 90. Stainless steel roast chamber full assembily

9.3 Bean Load Derivation

The ideal gas law where; p is gas pressure, V is gas volume, N is amount of gas particles in moles, k is the Boltzmann constant, and T is temperature.

$$pV = NkT$$

Heat is equal to temperature multiplied by Boltzmann's constant:

$$Q = kT$$

Rearranging heat can be expressed as the pressure times volume divided by gas number:

$$Q = \frac{pV}{N}$$

$$V = \frac{NQ}{p}$$

Volume flow f:

$$f = \frac{V}{t}$$

Heat flow $\dot{Q}$:

$$\dot{Q} = \frac{Q}{t}$$

Heat flow in terms of volume flow and pressure:

$$\dot{Q} = \frac{fp}{N}$$

Thermal resistance:

$$R_{thermal} = \frac{\Delta T}{\dot{Q}}$$

Thermal resistance expressed in terms of change in temperature difference, volume flow, pressure, and number of gas molecules:

$$R_{thermal} = \frac{\Delta TN}{fp}$$

The Bean load is equal to the difference between the loaded roasting chamber and the empty roasting chamber:

$$Bean\ Load\ = R_{thermal\ Loaded} - R_{thermal\ Empty}$$

Additionally, assuming the factors N, f,and p are the same in both cases the bean load can be written as:

$$Bean\ Load = \frac{N}{fp}\left(\Delta T_{load} - \Delta T_{empty}\right)$$

The exact bean load is calculable using this method however for the purpose of detecting change in a signal processing environment the important metric is reduced to: $Bean\ Load = \Delta T_{load} - \Delta T_{empty}$.