

A Thermodynamic Approach to Roasting Parameters and Stages of Roast

By Paul Songer

Roasting coffee is a thermodynamic process in which the application of heat and the resulting uptake of heat by the bean directly affects final flavor. The condition under which heat is applied is affected by environmental factors, including internal volume of the roaster, humidity, barometric pressure, and ambient temperature. The ability of the bean to take on heat and the rate at which the absorbed heat dissipates throughout the bean is a function of its physical state, including % moisture, density, and bean size. The chemical changes taking place at any instant in the process depend upon the amount of heat already taken on, the amount of heat available in the immediate environment, the ability of the mass of beans to conduct heat, and the reactions that have already taken place or are in the process of taking place. The roaster technician makes adjustments to the flame based upon knowledge of the roasting process, observations of the processes taking place, and experience.

In developing an understanding of coffee roasting, it is useful to examine the process from a thermodynamic perspective (where the main issues are heat and mass transfer) and from a flavor perspective (the chemical changes that take place as a result of heat application). Since what is occurring at any one point is dependent on what has previously occurred, this report will be organized on the basis of going through the roast process step by step, with particular emphasis on the specific issues posed and visual and auditory manifestations of the process.

The Roasting Process

The Thermodynamics of the Initial Phases of Roasting

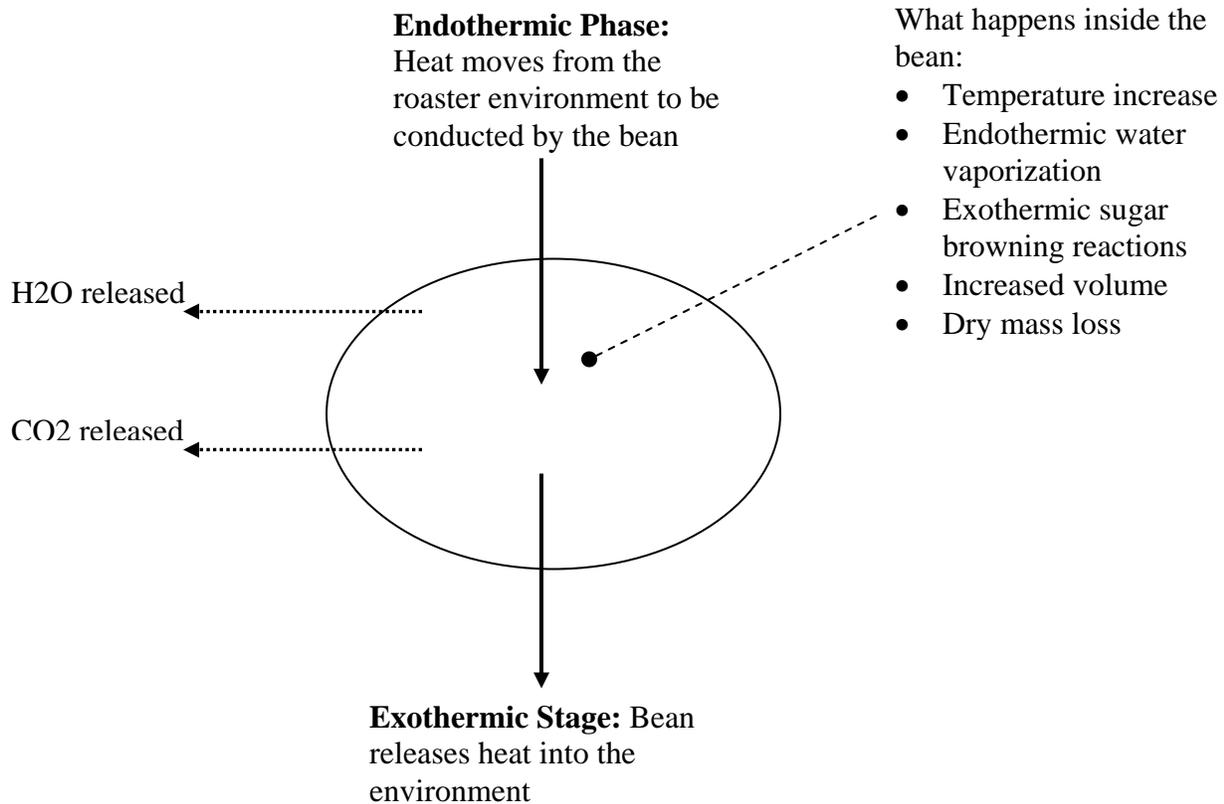
Thermodynamics is the study of energy, its transformations, and its relationship to the properties of matter¹. In visualizing thermodynamic models, it is useful to define the system under consideration and its

¹ Leland and Mansoori, Basic Principles of Classical and Statistical Thermodynamics, University of Chicago, p. 1.

boundaries. The system is loosely defined as that which inherently resists change. In this case, the system is defined as the mass of coffee being roasted. Heat transfer occurs from the roasting environment into the coffee across a boundary of zero thickness. The energy in the environment shapes the heat transfer across the boundary of the system. When the heat transfer is moving from the environment into the system, it is referred to as “endothermic,” heat absorbing; when heat is moving the opposite direction, from the system into the environment, it is referred to as “exothermic.”

The roaster controls the amount of heat being transferred by adjusting the amount energy in the form of heat in the environment (the roasting chamber). In the case under consideration, this is mainly accomplished by flame adjustment. A major challenge for any roaster is to anticipate the amount of heat that will be needed at certain roasting stages and adjust the flame accordingly. The amount of heat that will be applied to the roasting environment as the result of flame adjustment is affected by the amount of heat already present in that environment, the radiant heat present in the metal surrounding the chamber and from the drum, ambient humidity (air with higher humidity will not increase in temperature or dissipate heat as quickly), and ambient pressure (including the amount of air flow artificially induced by fans). These variations make every roasting environment unique.

The degree to which the system is able to be heated or is resistant to heat is called conductivity. The rate at which heat is transferred from the environment to the system depends on the amount of thermal energy present in the environment and how quickly the system is able to conduct the heat (heat capacity). In the case of coffee roasting, the heat initially moves from the roasting environment into the green bean, referred to as an endothermic reaction. As certain processes take place within the bean, the process gradually becomes more exothermic, releasing heat into the environment. The craft of roasting is based on anticipating these changes and making necessary adjustments. This process for roasted coffee is summarized in the diagram below².



When considering classic thermodynamic models, one assumes that heat originating in the environment is crossing a defined boundary into a system (endothermic) or from the system into the environment

² Diagram adapted from: Eggers and Pietsch, "Technology I: Roasting", Coffee: Recent Developments, 2001, Blackwell Science Limited, London, p. 90.

(exothermic). The system is most easily regarded as a group of rigid spheres with no mass transfer (only energy transfer) and conductivity that does not change. However, as can be seen from the diagram, during the roasting process the state of the system undergoes changes in terms of both mass transfer and direction of heat movement across the boundary. This necessitates the breaking up of the roasting process into stages that reflect the changes in conductivity, mass, and direction of heat transfer undergone by the system.

In considering these changes, it is important to review the Second Law of Thermodynamics. In a nutshell, this states that a thermodynamic driving force (heat, in this case) flows in one direction, from a system or environment that is hot to a system or environment that is cooler. When the temperature difference between two entities is large, the rate of change of temperatures is greater than when the difference is less. Heat is energy in transition and not a property of either the system or the environment. These phenomena are especially observable in coffee roasting, which utilizes large amounts of thermal energy (measured in Joules). Changes in thermal energy result in changes in temperature. For the temperature of a body to continue to rise, thermal energy must continue to be present or enthalpy (energy loss) will occur.

The first change that occurs within the bean is the heating of the green bean's surface moisture. Some of this moisture is vaporized (for this reason, this stage is referred to as "the drying stage"), collapsing the first layers of cells while some moisture heats the interior of the bean. The roaster observes this by noting expansion in size and a change in bean color.

The beans themselves influence the rate at which this takes place. The conductivity of the system is a function of the physical state of the green coffee. In washed process coffees, the bean moves from a green or blue-green to more of a jade green. Natural process coffees (such most Indonesian or Brazil coffees), which begin as pale yellow, deepen in hue to a golden color. The amount of swelling that takes place is an indication of how quickly the bean is taking on heat. This is partially dependent on the amount of moisture in the bean, which typically varies from 9-12%. Past crop coffees (including Central Americans purchased in the fall or

early winter) have less moisture and will not take on heat as quickly. Past crop coffees will not turn as richly green and may even fade slightly in the early stages of roasting. This is an indication that more heat will need to be applied over the entire roast period in order to effect the changes desired. The moisture present in the green bean acts as a heat conductor and if less moisture is present the bean will be more resistant to roasting. Since it can be assumed that there are also high humidity gradients caused by evaporating water that is moving into the roast gas, the thermal properties between the core and the surface of the bean are reasonably different³. At this point, not many observable chemical changes are taking place, but this stage may be important in the development of aroma precursors⁴. It is also important in determining how quickly the absorbed heat will distribute throughout the bean. It is possible to overheat the beans at this stage, burning and charring the outside yet not allowing a gradual enough heat penetration. Conversely, if not enough heat is applied (or, as often happens, if the mass of coffee, the “charge,” to be roasted is too large) the beans will not heat evenly. At this stage, a great deal of the thermal energy in the roaster is required for evaporation⁵, but little of that energy is applied towards roasting reactions. The “drying stage” is a preparatory stage and the amount of time it takes will determine the heat difference between the outside and center of the individual beans.

The expansion that takes place at this stage increases the porosity of the bean. What occurs at this point becomes especially important at the later stages of roast; greater porosity will result in decreasing volumetric heat capacity after moisture has been driven off and, especially, after first crack. Fast-roast techniques expand the bean to a greater degree and such coffees have greater porosity.

³ Hobbie and Eggers, “The Influence of Endothermic and Exothermic Energies on the Temperature Field of Coffee Beans during the Roasting Process,” 19th International Scientific Colloquium on Coffee, 2001, Association Scientifique du Café, Paris, p. 2.

⁴ Schenker, et al. “Impact of Roasting Conditions on the Formation of Aroma Compounds in Coffee Beans,” Journal of Food Science, Vol. 67, No. 1, 2002, Institute of Food Technologists, p. 65.

⁵ Hobbie and Eggers, “The Influence of Endothermic and Exothermic Energies on the Temperature Field of Coffee Beans during the Roasting Process,” 19th International Scientific Colloquium on Coffee, 2001, Association Scientifique du Café, Paris, p. 1.

With sufficient heating of the bean and the removal of a certain amount of surface moisture, the chemical changes associated with coffee roasting begin (referred to as “roasting proper” by Dr. Clarke⁶) and the coffee moves from gold/yellow into a brown or reddish brown phase. This process begins when the bean temperature is around 160° C⁷. This color change indicates that the sugar browning reactions have begun to take place. It is these browning reactions (which include Maillard reactions, caramelization, and other reactions) that gradually move the thermodynamic process from one of an endothermic reaction (heat absorbing) to an exothermic reaction (heat releasing). The “activation energy” at which the sugars begin exothermic chemical reactions is 175° C⁸. The amount and rate of this reaction is determined by the concentration and type of sugars present in the bean (higher quality coffees have a greater amount of sugar than lower quality coffees; past crop coffees have less sucrose but more glucose) as well as moisture content and ambient heat (the increasing bean temperature). This is one of the most important phases of roasting; the rate of roast and resulting chemical reactions will be established as the result of the amount of heat taken on and the rate of sugar browning reactions.

The change in the internal energy of the system at this stage is the sum of the heat entering the system from the environment and the heat being created by the sugar browning reactions. Like a snowball rolling downhill, the sugar browning reactions develop a momentum of their own and the increase in internal energy depends less and less on the heat in the environment as the roast progresses and more on the heat already taken on, the buildup of pressure within the bean, and the heat released by sugar browning.

Important observations to be made by the roaster at this point are color, color change, color uniformity, and the rate of color change. Excessive temperatures are to be avoided since the bean can only take on heat at a certain rate (this may be reflected by uneven splotching of dark brown/black colors on the bean). If the environment is too hot (or if the

⁶ Clarke, R.J., “Roasting and Grinding,” Coffee Volume 2: Technology, 1985, Elsevier Science, London, p. 79.

⁷ Eggers and Pietsch, “Technology I: Roasting”, Coffee: Recent Developments, 2001, Blackwell Science Limited, London, p. 90.

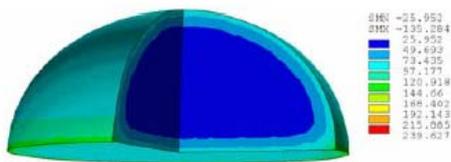
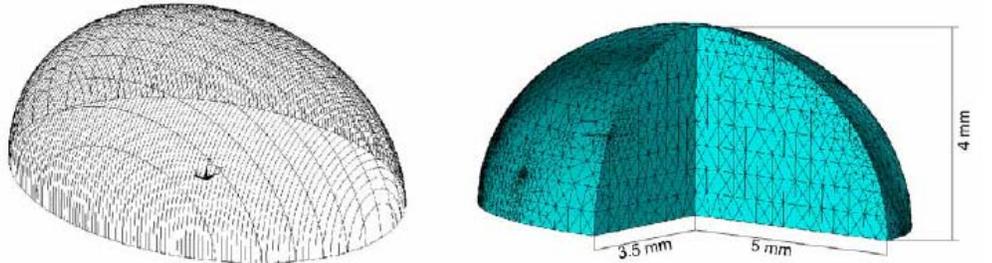
⁸ Hobbie and Eggers, p. 1.

beans are allowed to remain in contact with hot metal surfaces within the roaster for too long), the result is carbonization and charring of the bean surfaces. On the other hand, if the environment temperature is too low, the heat within the bean will dissipate, halting the roasting reactions.

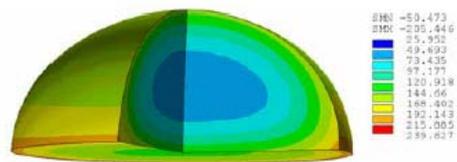
Besides color, an important clue to the roaster is the aroma of the coffee as it develops. A sourish green aroma, possibly somewhat like peanuts in natural process coffees, is the first to develop. As the coffee moves from golden to reddish-brown, a sweet-roasty aroma develops. Finally, the more familiar coffee aromas develop at a temperature of 180-190° C⁹. The smell of burning may indicate carbonization.

Hobbie and Eggers did a simulation of this process using a half-ellipsoid geometrical model to imitate the coffee bean shape. The conditions assume an environmental temperature of 240° C. and an average conductivity. This is reproduced below.

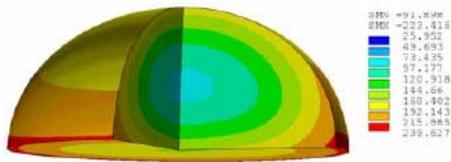
⁹ Schenker, et al. "Impact of Roasting Conditions on the Formation of Aroma Compounds in Coffee Beans," Journal of Food Science, Vol. 67, No. 1, 2002, Institute of Food Technologists, p. 60.



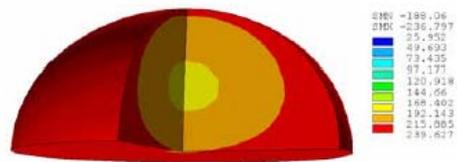
t=3 seconds



t=15 seconds



t=27 seconds



t=59 seconds

As can be seen, even with this relatively simple model the bean temperature is not uniform throughout the bean volume and is not steady throughout the roast. In addition, the charge is made up of different sized beans. This renders it difficult to determine an actual bean temperature. The best a roaster can do is measure the outer temperature of the bean and surmise the effect based on the process parameters. In addition to temperature, the gradual buildup of pressure inside the bean and gradually declining water content due to vaporization will affect the rate of heat conductivity.

In a controlled experiment conducted by Eggers, it was seen that the difference between the core and surface temperature was initially 70° C, while the difference between the core and half the distance to the surface was approximately 10° C¹⁰. Another observation made by Eggers was of

¹⁰ Eggers, R. "Heat and Mass Transfer during Roasting –New Process Developments," 19th International Scientific Colloquium on Coffee, 2001, Association Scientifique du Café, Paris, p. 7

“a small temperature drop suddenly appearing at a roasting time of 200 seconds. At this time the inner temperature differences are clearly higher in comparison to the outer temperature differences. However, the temperature course drops slightly simultaneously throughout the whole bean. After this unsteady phenomenon temperatures increase more rapidly than before! As an explanation one can assume a pressure built up in the center of the bean due to evaporating of water starting from the surface towards the central region but proceeding with decreasing velocity because the driving force of heat transfer – the temperature difference to the ambient – is diminishing all the time. So the pressure inside the bean increases until the temperatures overcome the vaporization temperature according to the pressure. Thus the remaining water in the center of the bean evaporates spontaneously and an endothermic flash creates the slight temperature drop.”¹¹

A further consideration is the influence of air movement within the roaster. This creates a change in pressure and convective heat and removes humidity and gasses and will affect the rate of the process, with greater airflow intensifying the effect of the applied heat.

The exothermic reactions climax with first crack. At this point, a great deal of heat is released into the roaster and considerable mass transfer from the roasting beans (in the form of moisture, CO₂, and other gasses) is taking place. Since the bean has expanded and loses mass during this process, it is considerably less dense and will not resist applied heat as easily. As a result, the batch is more subject to carbonization. The amount of exothermic energy released depends on the location, on the temperature, on the time a certain amount of organic compounds is being processed (reaction rate) and on the reaction enthalpy (heat loss as the result of the reaction).

At the point of first crack, the bean has already absorbed the potential heat energy that will produce the reaction. While the sugar browning reactions are occurring, the system is generating its own heat as well as

¹¹ Ibid.

absorbing heat. The exothermic energies lead to a further increase of the bean temperature without additional heat applied from the roast gas¹².

After first crack, the coffee has lost much of its mass and most of its moisture. As a result, the thermodynamic interaction between the system and the environment will change. Since the system has less mass, it is able to take on heat more quickly, but because it is less dense and has lost moisture it can also lose heat more quickly.

From a flavor perspective, the goal is to create a flavor profile made up of aromatics and a favorably perceived balance of sweet, acidic (tart), and sometimes bitter sensations, while minimizing the less appreciated astringent or bitingly bitter sensations. The purpose of roasting the coffee at a certain rate is not only to create the desirable flavors, but also to ensure a level of degradation of less desirable flavors.

The principle observable change is in the browning of sugar. In the “roasting proper” period before first crack, the sugars are heating up and some browning reactions are taking place. During first crack, the greatest amount of browning rates is taking place. At this point, many chemical pathways can be taken, especially in the presence of free amino acids (some of which are themselves the product of heating), which can result in a multitude of potential flavors. These flavors are the result of the temperature already attained by the reactants and the amount of thermal energy in the environment that is continuing to drive the process. The actual flavors themselves are partially the result of what is available in the bean for reaction, which specific amino acids and the form of the sugar (sucrose, glucose, or fructose). As a result, the roaster will find that some roaster profiles work better for some samples than another in emphasizing the unique attributes of a particular coffee. However, the flavor possibilities of browning reactions are almost infinite.

In addition to the sugar browning reactions, other reactions that will result in flavor are occurring. Perception of acidity (tartness) in the cup is due to a combination of several acids. During roasting, chlorogenic acid

¹² Hobbie and Eggers, “The Influence of Endothermic and Exothermic Energies on the Temperature Field of Coffee Beans during the Roasting Process,” 19th International Scientific Colloquium on Coffee, 2001, Association Scientifique du Café, Paris, p. 1

(which tastes a bit bitter and/or astringent) degrades into quinic acid and acetic acid is created as a by-product of sugar degradation. Certain carboxylic acids are inherently present in the green bean. Some do not degrade with roasting, such as lactic acid, while others such as citric and malic gradually degrade as the coffee darkens. The initial pH of green coffee is about 5.8. This drops to 4.8 (making the coffee more acidic) in the early stage of roast, and then gradually increases, with the darker roasts having the highest pH (least acidity).

Trigonelline is a nitrogen-based substance that is bitter in taste and degrades as the roast progresses. Carl Staub, inventor of the Agtron and roasting trainer, maintains that “For lighter roasts there will be more trigonelline, hence bitterness, but also less sugar caramelization. Caramelized sugar is less sweet in the cup than noncaramelized sugar, so when properly roasted these two constituents form an interesting compliment to each other.¹³” This is the basis of his “ideal reaction rate” –to balance the degradation of trigonelline with the caramelization of sugar (caramelized sugar tastes less sweet). Degradation of trigonelline begins at a temperature of 193° C and the majority has degraded by the time the batch reaches a temperature of 230° C, a moderately dark roast. Degradation products include the aromatic classifications of pyrroles and pyridines, characteristic of dark roast flavor profiles, and nicotinic acid, generally regarded as favorable.

As mentioned, the degradation of chlorogenic acid produces quinic acid, usually perceived as pleasantly sharp. In addition, caffeic acid, quinones other than quinic acid, and phenols are produced through chlorogenic acid degradation. Many roast measuring systems, including the Agtron, use the degree of degradation of chlorogenic acids as a means to measure roast degree (by measuring the amount of quinones present). Depending on roast degree, a certain amount of residual chlorogenic acids, generally perceived as more bitter or astringent, may still be present. The aforementioned phenols have the effect of drying the salivary glands and creating an astringent sensation.

¹³ Staub, Carl, “SCAA Roast Color Classification System,” 1995, Specialty Coffee Association of America, Long Beach, CA.

In comparison to most beverages consumed, coffee is not thought of as sweet and most of the sugar present in green beans is consumed by roasting reactions. However, lower than threshold amounts of sweet tasting substances will have a modifying effect on other flavor sensations experienced. Sugar is perceptively sweeter than caramelized sugar and caramelization increases with darkness of roast.

In addition to flavor (tastes and aromas together), an important aspect of coffee flavor is body, how the liquid feels in the mouth. This sensation is due to viscosity of the liquid and is influenced by different phases (oils, particles, etc.) dispersed throughout the beverage¹⁴. Perception of body is mainly due to the cellulose structure of the bean changing form and becoming more soluble as the result of applied heat. This cellulose is not soluble in the strict chemical sense of the word, but will extract as a solid suspended within the liquid. In a Newtonian liquid (one that obeys expected physical laws, such as flowing down hill, etc.), perception of body is due as much to uniformity of size of particles distributed through the liquid as amount of particles¹⁵. Other mouth sensations, such as astringency and presence of oil (especially in espresso preparations), may affect the perception of body. Light roasted coffees are quite thin and body increases as roast progresses and more cellulose is converted in form.

The final consideration in a flavor profile is taste sensation interrelationships. Higher acidity increases the perception of sweetness and bitterness¹⁶. It is up to the roaster to balance these in a way that will create the best flavor profile of the particular sample being roasted.

During second crack (which typically begins as the bean reaches a temperature of 230° C), the cellulose and other complex carbohydrates that compose the cell walls of the bean begin to fracture as the result of

¹⁴ Petracco, M. "Technology IV: Beverage Preparation: Brewing Trends for the New Millennium" Coffee Recent Developments, edited by Clarke and Vitzthum, 2001, Blackwell Science Ltd, London, p. 140.

¹⁵ Dr. Terry Acree, Dept of Food Science and Technology, Cornell University, Geneva N.Y., personal communication.

¹⁶Heath, H. B., "The Physiology of Flavor: Taste and Aroma Perception," Coffee Vol. 3: Physiology, edited by Clarke and Macrae, 1988, Elsevier Applied Science, London, p. 153.

heat¹⁷. The caramelization of sugars is fully accomplished by the time the coffee reaches 230-240° C and most of the carboxylic acidity has been volatilized. The primary consideration in terms of roasting at this level is maintaining the inherent structure of the bean while allowing the roast to progress.

The flavor profile has entirely shifted from the balance of sweetness, acidity, and bitterness to characteristic dark roast flavors dominated by bitterness. Since much of the soluble cellulose has volatilized, the sensation of body begins to reduce as roast progresses. Many aromatics volatilize completely and a few characteristic “dark roast” aromas dominate the aroma profile.

After second crack, there is danger of creating problematic unacceptable flavors due to overheating. If the heating is uneven, the cell matrix will be damaged, carbonization will occur unevenly, and the flavor quality of the coffee will be diminished. High levels of pyridine will adversely affect the flavor¹⁸. Earlier in the roast, trigonelline degrades into a mixture of pyridine derivatives¹⁹, some based upon combination with methyl and other alcohols (3-Methylpyridine, 4-Ethylpyridine, etc). Thermally induced methanol loss leaves pure pyridine, described as ashy and smoky in flavor²⁰. (The temperature at which this occurs was not given in the study evaluated.)

Under controlled conditions, the environment should never exceed 280° C and a safer temperature to maintain is about 270° C²¹.

Summary and conclusions: The roasting process is a thermodynamic process that involves manipulating the heat of the environment (the roasting chamber) in order to bring about chemical changes within the system (the mass of coffee). The success of the process is due to

¹⁷ Staub, Carl, “SCAA Roast Color Classification System,” 1995, Specialty Coffee association of America, Long Beach, CA.

¹⁸ Rizzi and Sanders, “Mechanism of Pyridine formation under Coffee Roasting Conditions,” 1996, *Flavour Science*, Vol. 197, p. 208.

¹⁹ Ibid, p. 209.

²⁰ Ibid, p. 208.

²¹ Staub, Carl, “SCAA Roast Color Classification System,” 1995, Specialty Coffee association of America, Long Beach, CA.

the final degree of roast, the time of roast, and the processes that have occurred as the result of application of heat. Response of the green beans that make up the system to the changes in heat is due to quality, its density, and moisture content. The physical factors of density and moisture content will change as the roast progresses. Each stage in the roasting process is dependent on the amount of heat already absorbed by the system and the roaster must anticipate the amount of heat that will be required. At all stages there is the possibility of losing the roast (allowing the system to exotherm too much of its heat) or burn, carbonizing and adding undesirable flavors to the roast.

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