

Basic Chemical Reactions Occurring in the Roasting Process

by Carl Staub

Many thermal and chemical reactions occur during the roasting process: decarboxylation, dehydration of quinic acid moiety, fractionization, isomerization, polymerization, and complex sugar reactions. The principal thermally reactive components are monosaccharides and sucrose, chlorogenic acids, free amino acids, and trigonelline. Both arabinose and galactose of polysaccharides are split off and the basic sulfur containing and hydroxyamino acids decompose. Carbohydrates both polymerize and degrade, liberating thermally unstable monosaccharides decomposing 20-30% of the polysaccharides, depending on the degree of roast.

Sucrose: Disaccharide of d-Glucosyl and d-Fructosyl Moieties

Sucrose is the principle sugar in coffee. The melting point of pure crystalline sucrose is in the 320-392 degrees F with 370 degrees F most commonly accepted. Degradation of dry sucrose can occur as low as 194 degrees F. and begins with the cleavage of the glycosidic bond followed by condensation and the formation of water. Between 338 and 392 degrees F, caramelization begins. It is at this point that water and carbon dioxide fracture and out-gassing begins causing the first mechanical crack. These are the chemical reactions, occurring at approximately 356 degrees F, that are exothermic. Once caramelization begins, it is very important that the coffee mass does not exotherm (lose heat) or the coffee will taste "baked" in the cup. A possible explanation is that exothermy of the charge mass interrupts long chain polymerization and allows cross linking to other constituents. Both the actual melting point of sucrose and the subsequent transformation, or caramelization, reaction are effected by the presence of water, ammonia, and proteinaceous substances. Dark roasts represent a higher degree of sugar caramelization than light roasts. The degree of caramelization is an excellent and high resolution method for classifying roasts.

Cellulose: A Long Linear Polymer of Anhydroglucose Units

Cellulose is the principle fiber of the cell wall of coffee. It is partially ordered (crystalline) and partially disordered (amorphous). The amorphous regions are highly accessible and react readily, but the crystalline regions with close packing and hydrogen bonding may be completely inaccessible. Native cellulose, or cellulose I, is converted to polymorphs cellulose III and cellulose IV when exposed to heat. Coffee's structure is a well developed matrix enhancing the mass uniformity and aiding in the even propagation of heat during roasting. Cellulose exists in coffee imbedded in lignocellulose (an amorphous matrix of hemicellulose and lignin containing cellulose), making up the matrix cell walls.

Hemicelluloses are polysaccharides of branched sugars and uronic acids. Lignin is of special note because it is a highly polymerized aromatic. Severe damage occurs to the cell walls of the matrix at distributed temperatures above 446 degrees F and bean surface temperatures over 536 degrees F. The actual temperature values will change due to varying levels of other constituents. Second crack, associated with darker roasts, is the fracturing of this matrix, possibly associated with the volatilization of lignin and other aromatics. Under

controlled roasting conditions, the bean environment temperature should never exceed 536 degrees F. A wider safety margin would be achieved by limiting the maximum environment temperature to 520 degrees F. These temperature limits minimize damage to the cell matrix and enhances cup complexity, roasting yield, and product shelf life.

Trigonelline: A Nitrogenous Base Found in Coffee

Trigonelline is 100% soluble in water and therefore will end up in the cup. Trigonelline is probably the most significant constituent contributing to excessive bitterness. At bean temperatures of 445 degrees F, approximately 85% of the trigonelline will be degraded. This bean temperature represents a moderately dark roast. 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. Trigonelline melts in it's pure crystalline form at 424 degrees F Degradation of trigonelline begins at approximately 378 degrees F.. The degradation of trigonelline is one of the key constituent control flags for determining the best reaction ratio.

Quinic Acid: Member of the Carboxylic Acids Group

Quinic Acid melts in pure crystalline form at 325 degrees E, well below the temperatures associated with the roasting environment. Quinic Acid is water soluble and imparts a slightly sour (not unfavorably as in fermented beans) and sharp quality, which adds to the character and complexity of the cup. Surprisingly, it adds cleanness to the finish of the cup as well. it is a stable compound at roasting temperatures.

Nicotinic Acid: Member of the Carboxylic Acid Group

Nicotinic Acid melts in pure crystalline form at 457 degrees F. Naturally occurring Nicotinic Acid is bound to the polysaccharide cellulose structure. Nicotinic Acid is also derived in soluble form during roasting. Higher levels of Nicotinic Acid for any given degree of roast are associated with better cup quality. Since it is 100% soluble, it will end up in the cup. Nicotinic Acid contributes to favorable acidity and clean finish. It's derivation rate is one of the key constituent control flags for determining the best reaction ratio temperature and chemistry propagation rates. Additionally, the interaction of melted Nicotenic Acid with other constituents contributes significantly to the intensity associated with darker roasts.

Environment Temperature

The temperature of the roasting environment determines the specific types of chemical reactions that occur. There is a window of temperatures that produce favorable reactions for the ideal cup characteristics. Temperature values outside of this window have a negative effect on quintessential cup quality. Even within the window values, different temperatures will change the character of the cup, giving the roaster the latitude to develop a personality or style desired, or to tame the rough signature of certain coffees while still optimizing relative quality. System Energy: At any given environment temperature, the amount of

energy (BTU) and the roasting system's transfer efficiency will determine the rate at which the specific chemistry will occur. Higher levels of both energy and transfer efficiency will cause the reactions to progress more quickly. There is a window of reaction rates that will optimize cup quality. This is called the Best Reaction Ratio, or BRR.

Best Reaction Ratio (BRR)

The best cup characteristics are produced when the ratio of the degradation of trigonelline to the derivation of Nicotinic Acid remains linear. The control model of this reaction ratio is a time/temperature/energy relationship. The environment temperature (ET) establishes the pyrolysis region for the desired chemical reactions while the energy value (BTU) and system transfer efficiency (STE) determines the rate of reaction propagation and linearity of Nicotinic Acid derivation to degradation of trigonelline. Because green bean density varies dramatically, under any given ET / BTU / STE format, the reaction distribution will vary. It takes longer to obtain comparable uniformity for a higher density bean. Monitoring the bean temperature offers a good method of approximating the reaction distribution during this phase of the roasting. The ideal environmental temperature, ET, for best reaction ratio, BRR, is from 401-424 degrees F, with 405 degrees F as the default value. The BTU required is determined by the system's transfer efficiency, or ability to impart the energy to the charge mass.

Maximum Environment Temperature (MET)

Establishing the thermal environment protocol for the ideal roast is a balancing act. While it is desirable to maintain the BRR temperature and energy levels until the target reactions are achieved, the BRR temperature is well above the caramelization temperature of sucrose. Because many roasting systems exhibit thermal hysteresis using simple temperature regulating schemes, care must be taken not to allow the coffee mass to exotherm. Additionally, limiting the maximum environment temperature, MET, is also important. As previously mentioned, maintaining structural integrity of the cellulose matrix is of great importance. Lower temperatures will reduce surface evaporation of constituents minimizing the capillary action that draws constituents to the surface where they would be volatilized. Hydraulic action, a function of internal pressure which is directly related to bean temperature, is already at work. By limiting the maximum temperature, losses will be minimized and the essence of coffee retained. Consequently, the MET should not exceed 520 degrees F. This roasting system bases the MET value on the actual final bean, or drop temperature, which correlates to the degree of roast.