

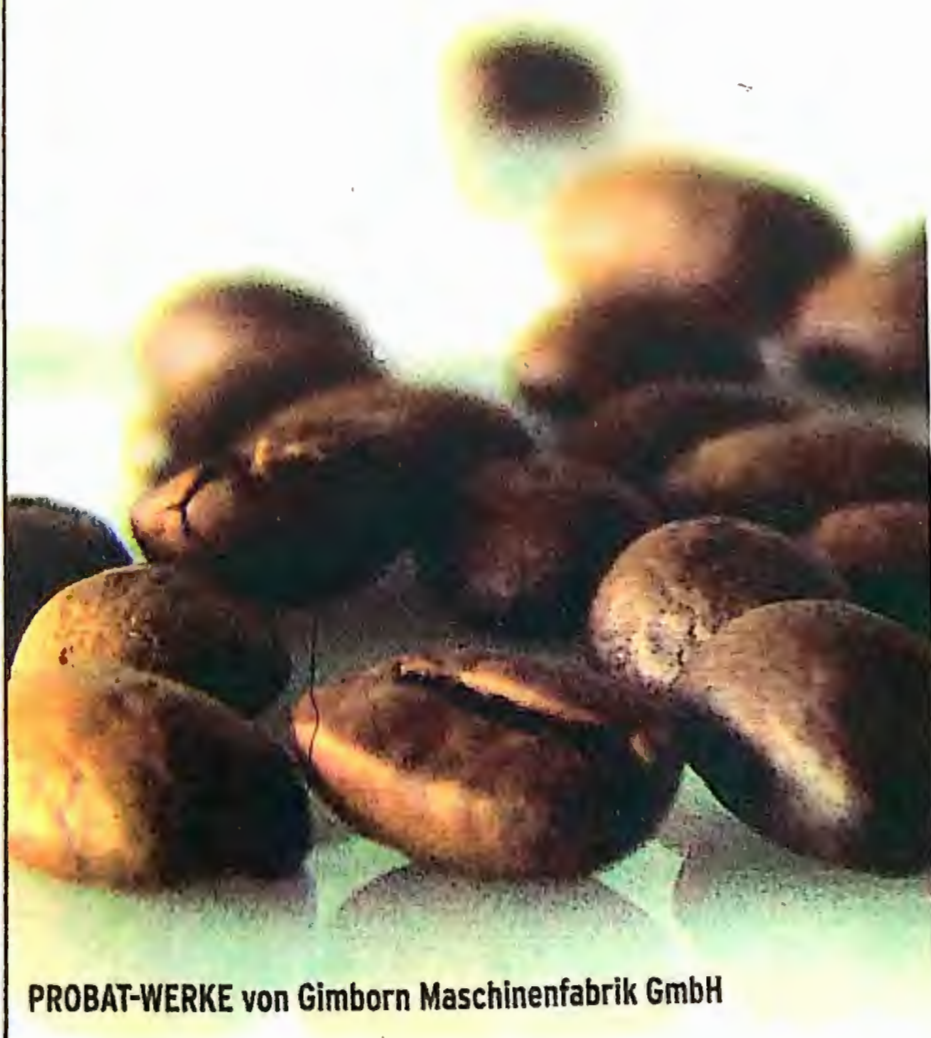
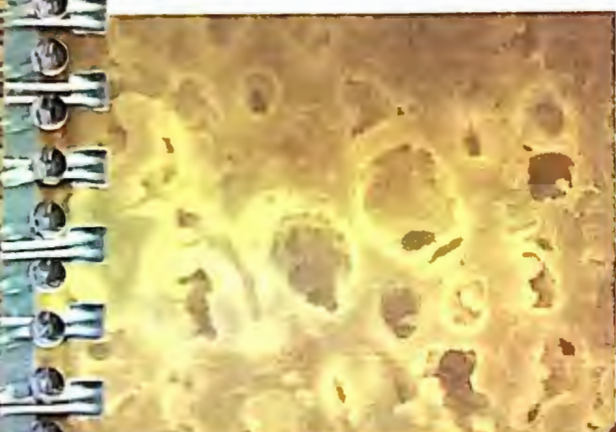
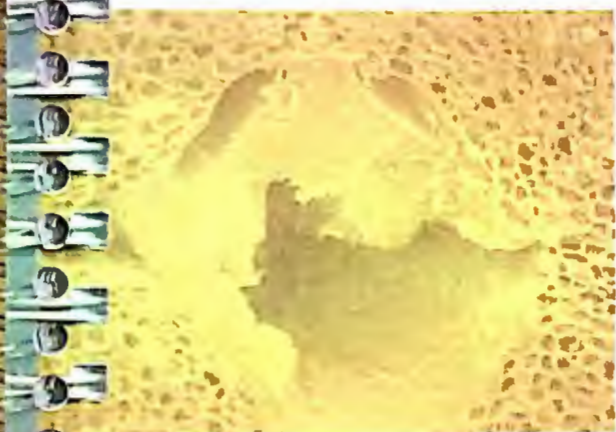
Gerhard A. Jansen

# COFFEE

# ROASTING

Magic - Art - Science

Physical changes and chemical reactions



PROBAT-WERKE von Gimborn Maschinenfabrik GmbH

A stanza from the coffee cantata:


## KEEP QUIET, DON'T PRATTLE

4th aria (soprano): Liesgen

Ah, how sweet coffee tastes!  
Lovelier than a thousand kisses,  
smoother than muscatel wine.  
Coffee, coffee, I must have it,  
and should anyone wish to give me a treat,  
ah! just pour me some coffee!

Music: Johann Sebastian Bach, 1734/35  
Text: Christian Friedrich Henrici (Picander), 1732



Three coffee beans are shown at the top of the page. One bean is in the foreground, slightly to the right, showing its characteristic shape and color. Two other beans are in the background, one to the left and one to the right, slightly out of focus. The beans are dark brown with some lighter, yellowish-brown areas, suggesting they are roasted.

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# 1 FOREWORD

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This handbook contains the wealth of experience gained by the R&D department of PROBAT-WERKE, Emmerich, with regard in particular to the physical and chemical processes that take place during coffee roasting.

The subject matter is intended to stimulate interest in this complex field and to promote knowledge about the product for the processing of which the facilities and machines at the PROBAT-WERKE are developed, constructed, manufactured and sold.

This handbook is not intended as a textbook, but rather for looking up individual subjects and terms. The compact compilation of what is worth knowing and the easily understandable explanations are illustrated by means of figures and images.

**Emmerich on the Rhine**  
**November 2006**

**Gerhard A. Jansen**



# CONTENTS

1	Foreword	3
2	About the author	5
3	Introduction	6
4	Green coffee	8
5	Roasting process	14
5.1	General information	14
5.2	Temperature	17
5.3	Thermal energy	20
6	Physical changes	22
6.1	General information	22
6.2	Form/structure	23
6.3	Color	28
6.4	Volume	30
6.5	Weight loss	34
6.6	Density	38
6.7	Dehydrolysis	40
6.8	Oil migration	45
7	Chemical reactions	46
7.1	General information	46
7.2	Maillard reaction	48
7.3	Pyrolysis	51
7.4	Hydrolysis	62
7.5	Conversion into caramel	64
7.6	Oxidation	64
7.7	Decarboxylation	65
8	Coffee beverage	68
9	Reflection	69
10	Appendix	70
10.1	Graphics index	70
10.2	Literature	72



## 2 ABOUT THE AUTHOR

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Gerhard A. Jansen was born in 1944 in the Netherlands. He entered the company PROBAT-WERKE in 1970 as a design engineer in the field of roaster construction. In 1972, the R&D department was spun off from the technical department to be run as an independent division. Jansen participated in building up the division, ran the technical office there until 1966 and was the representative of the division's head. From 1997 to 2000 he was the company's manager for process engineering and applications technology. Since 01.01.2001, Gerhard A. Jansen has been running the R&D department and is the authorized signatory of the company PROBAT-WERKE in Emmerich on the Rhine.

PROBAT-WERKE designs, constructs, manufactures and sells facilities for the coffee processing industry worldwide. Its main pursuit in the area of research and development concerns the engineering aspects of coffee processing, with a focus on roasting and grinding. PROBAT-WERKE enjoys a particularly good reputation among the mechanical engineering companies that manufacture coffee roasting facilities because the company is also involved with the product to be processed with their machines and maintains a large laboratory in this regard.

By virtue of his activities, Gerhard A. Jansen, who is currently in charge of this R&D laboratory, can fall back on extensive experience based on both the technical as well as analytical aspects of coffee processing.

# 3 INTRODUCTION

When drinking a cup of coffee, practically every sense available to man is activated. The multi-faceted aromatic smell, the mild acid and the pleasantly bitter taste in the oral cavity, as well as the sensation or touch on the lips, tongue and gums, the gold-brown, creamy appearance of the beverage, and not least of all the experience of its aftertaste and stimulating effect, all contribute to the wonderful experience of enjoying a coffee.

Although nature itself gives us coffee in its original form with many different, sort-related qualities, it challenges mankind to discover the hidden properties and to cultivate them.

The terms used in the title — “magic”, “art” and “science” — are not new in the context of coffee processing. Yet although they have already been used by several authors, they are nonetheless still the best description of the fascinating process of roasting coffee.

The act of transforming pale, unpleasant smelling raw coffee beans into wonderfully brown, aromatic and tasty roasted coffee is indeed a feat of magic. Roasted coffee affects us like an object of art — it radiates preciousness. The process control required for the optimal completion of this procedure with regard to quality and economy is hardly possible without the support of science.

**To recapitulate: The roasting of coffee is at the same time**

- **MAGIC**
- **ART**
- **SCIENCE**



In this book the physical and chemical processes arising in the roasting procedure will be presented in a way that is clear and comprehensible, however, before dealing with the subject of "Physical changes and chemical reactions when roasting coffee", it is absolutely necessary that the raw product first be given a brief introduction.

Green coffee is a natural product. Like everything that grows naturally, every single coffee bean, when all is said and done, has its own individual features. This fact always has to be taken into account when treating this raw material and setting demands for the end product. Despite every aspiration towards uniformity in appearance and quality, the individuality of the green bean will nonetheless remain recognizable. It is nature itself that sets a limit on human intervention.

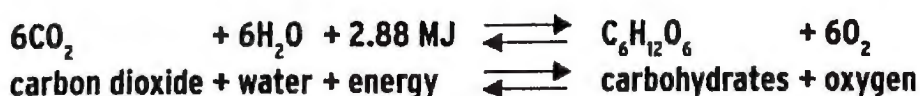
# 4 GREEN COFFEE



Green coffee with its characteristics is the foundation upon which the roasting process is based. The prerequisite for a specific end quality of coffee is the proper interplay between the types or blends of green coffee used and the roasting process.

The cultivation of coffee is greatly dependent on geographical and climatic circumstances. Soil composition and altitude as well as temperature, light conditions and precipitation contribute to the yield and qualitative properties of the coffee. Moreover the yield and quality is considerably influenced by measures taken on the plantation with respect to protection and plant husbandry.

The basic modules necessary for development must be perfectly coordinated. Responsible in general for the growth and development of the plants is photosynthesis, whereby carbon dioxide and water are converted into carbohydrates. The energy required for this is drawn by the plants from sunlight. In this multistage reaction, the plant releases oxygen. The following equation is a simplified representation of this process.



The many different carbohydrates, lipids and proteins which are formed are responsible for the quality of the coffee. Alongside this basic metabolic process a formation of secondary substances takes place which, for example, can be indispensable for the survival of the plant. Among these secondary materials which are present in more or less low quantities in the coffee plant are caffeine, trigonelline and chlorogenic acids. Caffeine, for instance, acts to



protect the coffee plant against mold formation and simultaneously stems the formation of mycotoxins. It is assumed that the unsavory chlorogenic acids keep the plant from being eaten by animals. The minerals indispensable as building materials, mainly potassium, are present in green coffee, although the quantities are only negligible.

“Carbohydrate” is a collective term for many chemical compounds composed of carbon, hydrogen and oxygen atoms. Carbohydrates are subdivided into monosaccharides, i.e. simple sugar, such as, among other things, glucose and fructose; oligosaccharides such as sucrose; and polysaccharides, such as, among other things, arabinogalactan, celluloses, mannanes, starches and pectins.

According to the type of green coffee and its area of cultivation, different constellations of individual substances and correspondingly diverse qualities can be expected. There are three types of green coffees:

- **Coffea Arabica**
- **Coffea Canephora, known as Robusta**
- **Coffea Liberica**

Liberica coffee is less appreciated due to its acrid taste and has hardly any economic significance.

Arabica coffees are highland coffees cultivated at altitudes above 1000 m. The higher the plantations, the slower the fruit ripens and the heartier and fuller the taste of the coffee is. The altitude of the region of coffee cultivation is synonymous with the grade of coffee quality.

## 4 GREEN COFFEE

Robusta coffees are cultivated in areas below 1000 m. Robusta coffees are generally distinguished from Arabica sorts through the form and appearance of the beans and through the less appealing taste. Fullness – or body – in the cup is, particularly for Robustas, a given.

Within these types of coffees, the different types of raw coffees are sorted according to country and/or region of origin. Each sort is made up of its own specific individual substances, which can lead to quite specific profiles as regards aroma and taste.

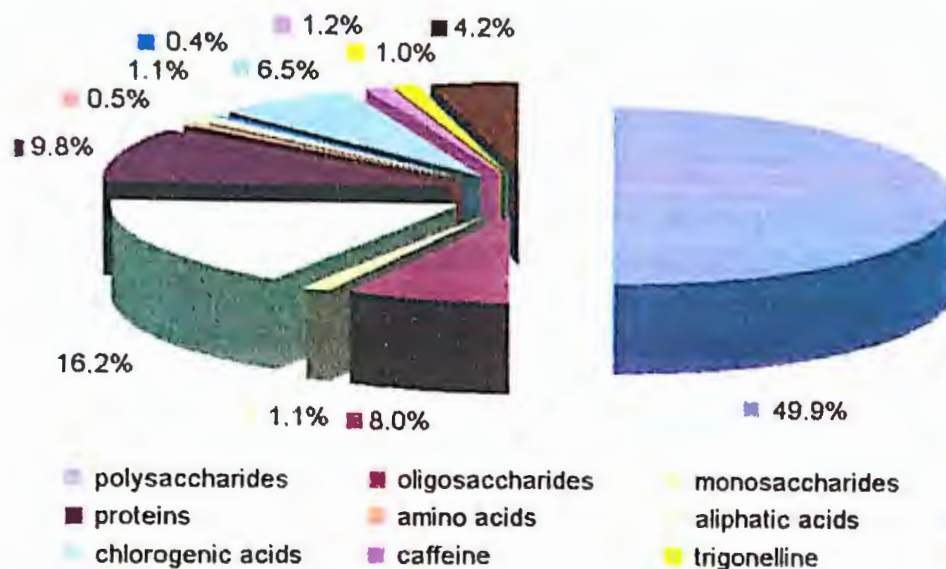
The chemical composition for a very specific Arabica (Fig. 1) and a very specific Robusta (Fig. 2) green coffee is portrayed in the pie charts in % dry substance.

The total share of carbohydrates amounts to more than half of all of the constituent substances. What is remarkable are the different proportions of lipids, chlorogenic acids and caffeine in Arabica and Robusta green coffees. Compared to the Robusta coffee sorts, Arabica coffees have a greater proportion of lipids with 16.2% against 10% and, with 6.5% against 10%, less chlorogenic acids. The 1.2% caffeine content of Arabica coffee is considerably less than the 2.2% of Robusta coffee. At 8%, the sucrose content of Arabica sorts is substantially higher than Robusta's 4%.

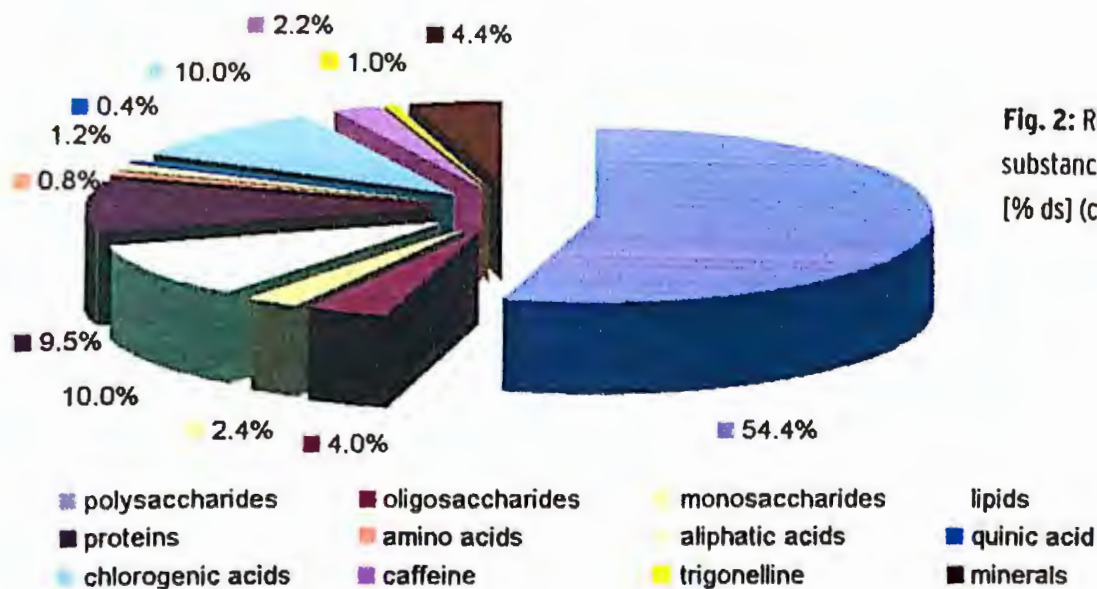
In the R&D department of PROBAT-WERKE, the following content percentages were analyzed in the green coffee for both coffee types.

	Arabica	Robusta
Lipids (fat)	13.0 - 17.0%	7.0 - 10.0%
Chlorogenic acids	5.8 - 7.7%	6.8 - 10.0%
Caffeines	1.0 - 1.7%	2.2 - 3.4%

The preparation of coffee beans for transport and storage likewise influences the quality of the product. Two methods are known: dry processing and wet processing. The dry or natural processing is employed mainly in regions with high yields and suitable climatic conditions such as, for example, Brazil. In regions with too little sunshine, wet processing is carried out. The wet-processed coffee beans are called "milds" in international trade. These washed coffees have a greater, more pleasant share of acids than dry-processed coffees. Robusta sorts are mostly dry processed.



**Fig. 1: Arabica - Chemical substances in green coffee [% ds] (cf. Illy and Viani, 1995)**



**Fig. 2: Robusta - Chemical substances in green coffee [% ds] (cf. Illy and Viani, 1995)**

The water content of green coffee beans is approx. 8% to 13%, as a rule between 10% and 12%. At water contents above 13.5%, there is a danger that the beans become musty or moldy. Moreover at higher moisture levels, a subsequent fermentation can take place.

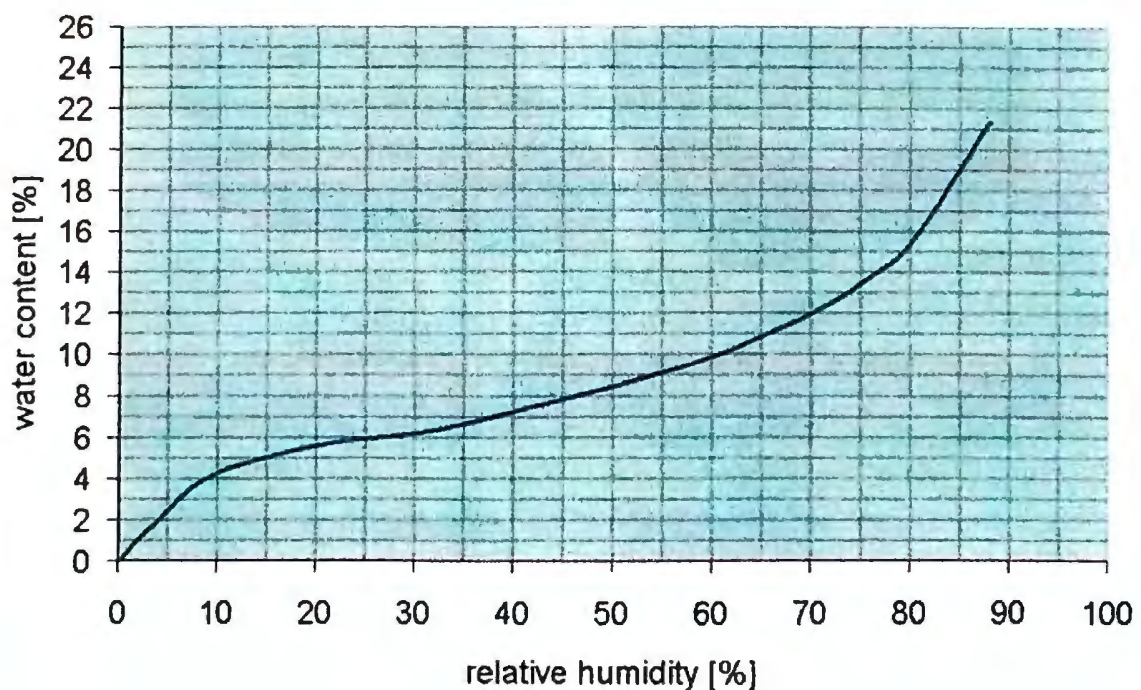
## 4 GREEN COFFEE


The mold limit lies at a relative atmospheric humidity of 75%. With a green coffee water content of approx. 13.5% and a relative atmospheric humidity of 75%, both are balanced. An exchange of moisture between coffee beans and ambient air will no longer take place. The relation between the water content of raw coffee and a relative atmospheric humidity arises from the sorption isotherm for a temperature of 20°C (Fig. 3).

The green coffee qualities are evaluated according to form, size, bean symmetry, color, horniness, shell, cut, luster, bean surface smoothness, proportion of failed beans, foreign elements and odor.

Evolution on the one hand and centuries of knowledge accrued by coffee cultivators on the other hand have led to today's quality of coffee beans. Until now, nature, supported by man, has been able to allow the ripening process of coffee beans to run its course undisturbed. The result is the variety of types and the increased resistance of the coffee plants.

Of course, by manipulating the natural circumstances, certain features or functions of a plant and thereby the chemical composition of the coffee bean can be altered. Scientific research and gene technology in particular are sub-





ject to hardly any limitations at present. To enter into a discussion on whether genetically altered coffee offers economical or qualitative advantages or disadvantages, whether genetically altered coffee sorts keep in the long term and what is expected of them would exceed the bounds of this book. The fact of the matter is that the composition of the individual substances, whether left natural or manipulated, influences the aromatic compounds that result from roasting.

It should be emphasized here that although the coffee is treated and is run through a process chain with different stations, as a rule there are no foreign chemical substances added to it. What we know as coffee beverage is based entirely on the substances in the bean itself. Every chemical process during treatment is dependent on what nature has given the raw coffee bean. It is only this that will be dealt with in this chapter. The possibility of adding artificial flavors to the coffee or of subjecting the raw coffee to a pretreatment such as, for example, decaffeination or steaming will only be mentioned peripherally here and will not be looked into more closely in the subsequent consideration of the chemical reactions during roasting.

Although some stimulating substances are already present in green coffee, the woody- or "grassy"-tasting and musty-smelling, pale-looking product is unpalatable in its raw form. The basic substances required for making an exquisite beverage out of green coffee, although on hand, need the roasting process to develop, to set them free in the desired manner.

# 5 ROASTING PROCESS



## 5.1 GENERAL INFORMATION

In this handbook subtitled "Physical changes and chemical reactions", product data, numerical values and connections will be frequently mentioned and likewise portrayed in different forms which are based on experience and likewise have been calculated or analyzed. At this point it should be made clear and binding for the entire book that the results given here have been gathered, documented and assessed by the R&D department of PROBAT-WERKE and are made available to the general public in the framework of this book. In a few exceptions, developments from other sources are adopted and indicated accordingly.

The numerical values used for roasted coffee in the figures always refer to very specific coffee sorts roasted over a very specific time at a very specific roasting degree.

When coffee is roasted, a series of complex physical and chemical processes take place whereby the color, taste and flavor substances specific to roasted coffee are formed. The roasting process is one of the most important steps in the process on the way from green coffee to the tasty coffee beverage. Arising from a few initial chemical compounds during the roasting process are numerous volatile aromatic compounds.

The roasting process produces a dry and brittle texture which facilitates a crushing of the coffee beans and increases the extraction capability.

Coffee is roasted by a dry heating process which, unlike what is usual for many other natural products, is terminated at relatively high temperatures of up to 250°C. The transmission of heat to the surface of the coffee beans takes place by means of convection, radiation and contact. Heat conduction



inside the beans progresses from the outside inwards. The most important parameter in the roasting process is the specific quantity of thermal energy made available to the coffee beans. The coffee temperature profile, i.e. the course of the coffee temperature throughout the roasting time, is dependent on it. Decisive for the homogeneous roasting result for every single bean, as well as for the physical changes and for the chemical reactions, is the coffee temperature profile.

The roasting degree, i.e. the color of the roasted coffee, has an essential influence on the formation of aroma and development of the flavor, and is thus mainly responsible for the quality of the roasted product and ultimately the coffee beverage. Moreover, the roasting time has an influence that is not to be neglected. A satisfactory assessment based on the roasting degree without knowing the roasting time is – if at all – hardly possible.

Essentially, the roasting time and roasting degree of the coffee determine the coffee temperature profile. During the roasting time, the course of the coffee temperature profile can be influenced within a limited framework by specific adaptation of the amount of thermal energy.

Darker degrees of roasting tend to yield higher extraction concentrations, less acids, more body and more bitter substances. The residual water content is less. Short roasting times result in greater extraction contents, roasted coffee beans of greater volume, more overall acid and more bitter substances. A greater amount of water remains in the roasted coffee.

Once the desired roasting degree is reached, the coffee is cooled. As a rule, the hot coffee beans are cooled by means of ambient air. In the industrial process, the fully roasted coffee is in many cases quenched with water prior to the actual air cooling. Water-quenching, once the roasting process reaches

## 5 ROASTING PROCESS

a specific product temperature or coffee color, brings the roasting procedure to an abrupt stop. This assures that uniform and reproducible roasting degrees are achieved from charge to charge as well as within the charges. The side effect that the addition of water can result in an increased moisture content in the roasted coffee is used in many cases to obtain very specific roasted coffee moistures.

The distribution of moisture in the coffee bean is very important for the subsequent grinding procedure. Certain periods of rest between the roasting/cooling procedure and the grinding must be observed in particular with greater residual water quantities in the roasted coffee. In PROBAT roasting facilities, water-quenching takes place in the roaster itself, i.e., at a high ambient temperature. This has a positive effect on the distribution of water and on the transport of water into the coffee. The rest or compensation time of the roasted and cooled coffee beans can be reduced to a minimum. The degree of moisture naturally has an influence on the required hold time. To moisturize the coffee beans to the limit value of  $\leq 5\%$  prescribed by German law, for instance, a compensation time of about 2 to 4 hours is sufficient, depending on coffee sort and roasting degree.

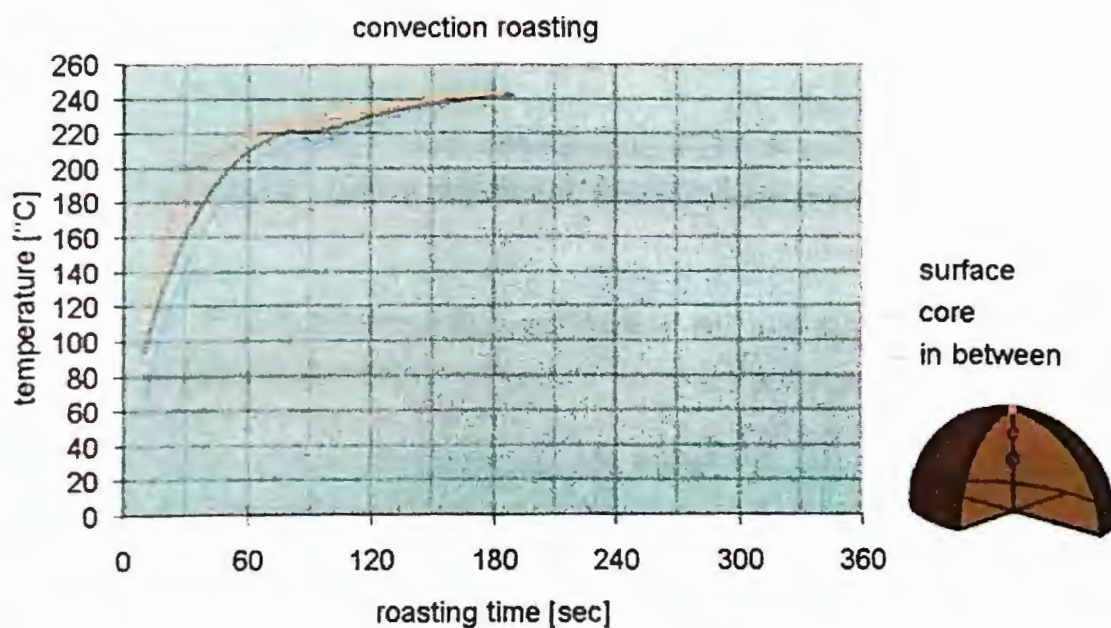
The cooling process following the roasting process is inseparably linked to the roasting process. In this chapter the effects of cooling on the quality of the coffee will not be gone into any further. It is, however, remarkable that hardly any scientific research has been done on the effect of cooling and that it receives little attention in reference works.

It is quite natural that the roasting process has to be terminated and that the coffee beans have to be cooled for storage and for a possible crushing step. Tests concerned with the temperature of the cooled coffee deal mainly with the influence of these temperatures on the oxidation behavior, i.e. the ageing of the coffee. Ground coffee in particular has been tested in this regard.

## 5.2 TEMPERATURE

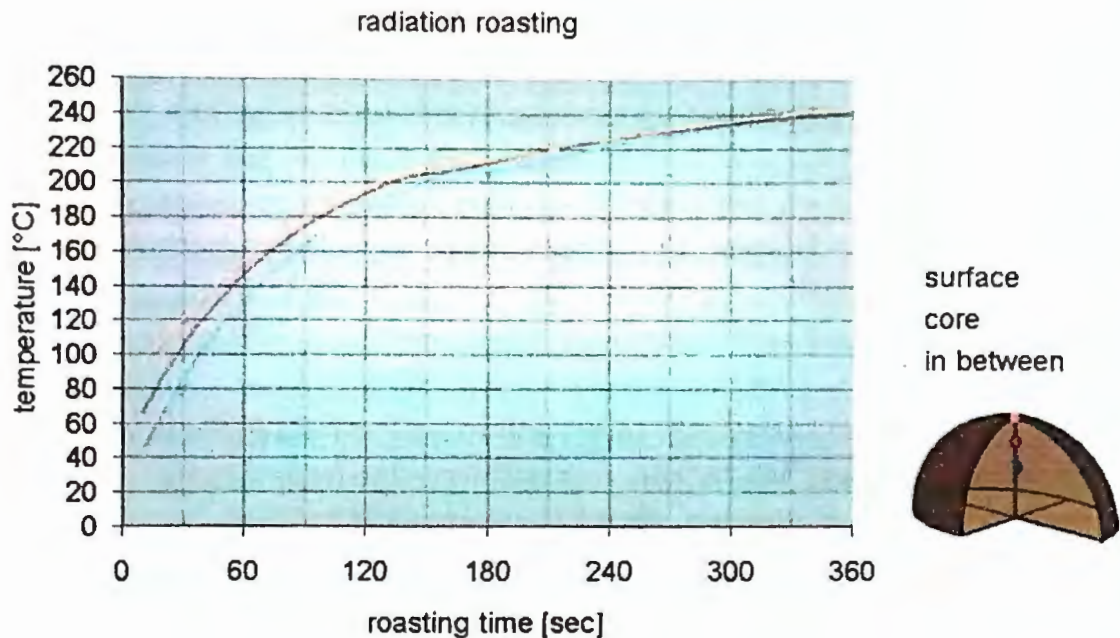
The heat transfer in the coffee bean progresses from the outside to the inside, the transport of the mass of volatile compounds inversely from the inside to the outside. This leads particularly in the initial phase of the roasting process to great differences in temperature of up to approx. 50°C between the outer and inner bean layers. Only at a bean core temperature of approx. 150°C do the temperatures gradually approximate one another.

The following figures (Fig. 4 and Fig. 5) show the bean surface temperature, the core temperature and the temperature between them for different coffee temperature profiles.



**Fig. 4:** Temperature development of a coffee bean  
[cf. Eggers, von Blittersdorff, Hobbie (2002), and Eggers (2001)]

# 5 ROASTING PROCESS



**Fig. 5:** Temperature development of a coffee bean  
[cf. Eggers, von Blittersdorff, Hobbie (2002), and Eggers (2001)]

A bean surface temperature of  $200^{\circ}\text{C}$  was determined after 36 seconds for convection roasting and after 125 seconds for radiation roasting. With  $43^{\circ}\text{C}$ , the temperature difference between surface and center for the faster temperature rise was substantially higher than for the slow rise, for which a temperature difference of  $10^{\circ}\text{C}$  was determined. The temperatures at the surface and in the core came closer to one another in the further course of the roasting process. At a bean surface temperature of  $220^{\circ}\text{C}$  the temperature difference reduced from  $43^{\circ}\text{C}$  to  $24^{\circ}\text{C}$ , and from  $10^{\circ}\text{C}$  to  $5^{\circ}\text{C}$ , respectively.

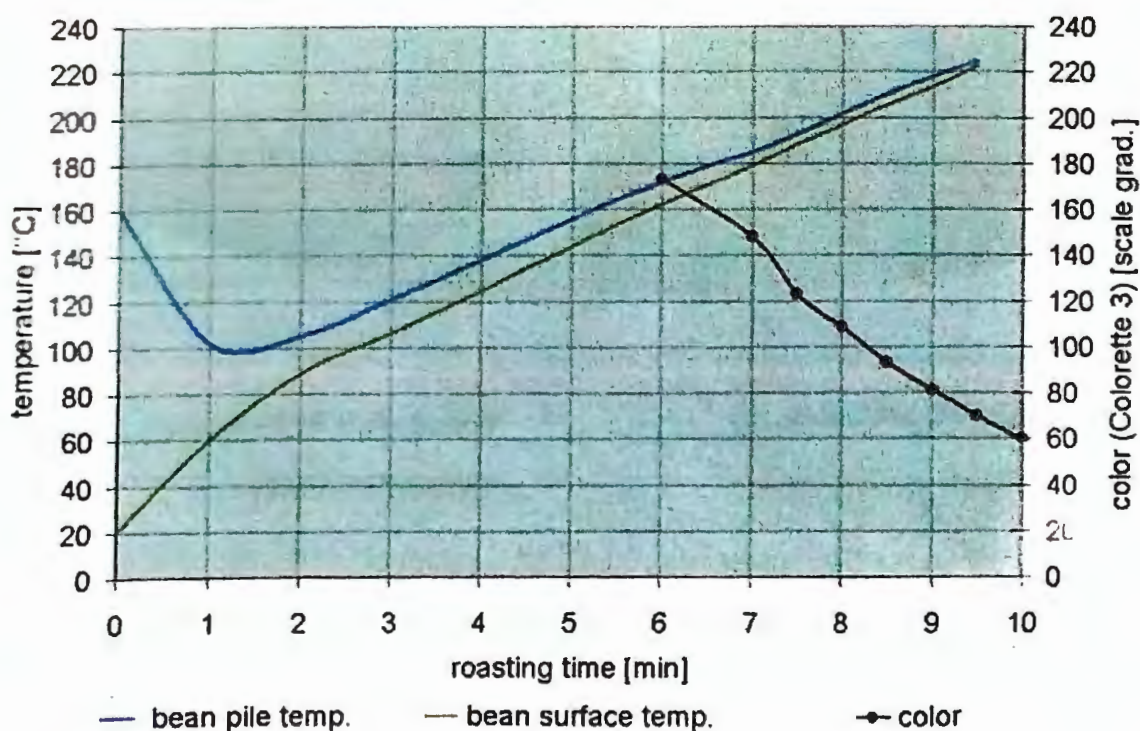
To be taken into account is that the bean surface and core temperatures shown here are the results of laboratory tests. In this case, coffee beans were roasted singly in a warming cabinet prepared especially for this purpose.

Normally, many coffee beans are roasted at the same time in a roasting bin. The smallest charge of approx. 700 coffee beans is processed in a sample roaster. The RN 5000 industrial roaster is filled with some 5 million coffee beans per charge. Contact between the individual coffee beans as well as contact of the beans with the walls of the bin have an effect on the trans-

fer of heat. The fact is that the time in which the coffee is roasted or the rise of the coffee temperature substantially influences the difference between the coffee bean surface and coffee bean core temperatures. The shorter the roasting time, the greater is this temperature difference.

In industrial use, for practical reasons the bean pile temperature is measured and used for controlling and directing the roasting process. The bean pile temperature is comprised of the surface temperature of the coffee beans on the one hand and the ambient temperature on the other. Hence the bean pile temperature does not provide precise information on the absolute temperature of the bean surface. A comparison of this coffee temperature is possible only up to a certain point due to many influences such as coffee sort, bean size, roaster type, i.e. roasting bin design, fill factor, position and type of thermocouple.

The following figure (Fig. 6) shows an example of the courses of the coffee temperatures during the roasting process. The graphic portrayal is only intended to give an impression and naturally refers only to a very specific roasting process with very specific process parameters.



**Fig. 6:** Temperature development during roasting

# 5 ROASTING PROCESS

## 5.3 THERMAL ENERGY

The thermal energy required for a specific coffee temperature profile is heavily dependent on the coffee sort, the roasting degree and in particular on the water content of the raw coffee. The thermophysical properties of the coffee beans, such as temperature conductivity, thermal conductivity and heat capacity, change constantly during the roasting process owing to the different physical properties.

The following pie chart (Fig. 7) shows an example of the theoretically calculated heat energy values for roasting Arabica coffee related to a very specific roasting degree based on 11.5% green coffee moisture. The energy released in the exothermal phase has been taken into account accordingly. The result of this is a specific heat energy requirement of 470 kJ per kg of green coffee. The proportion of exothermal heat used in this regard is roughly estimated. Precise statements on exothermal heat when roasting are not available at this point in time.

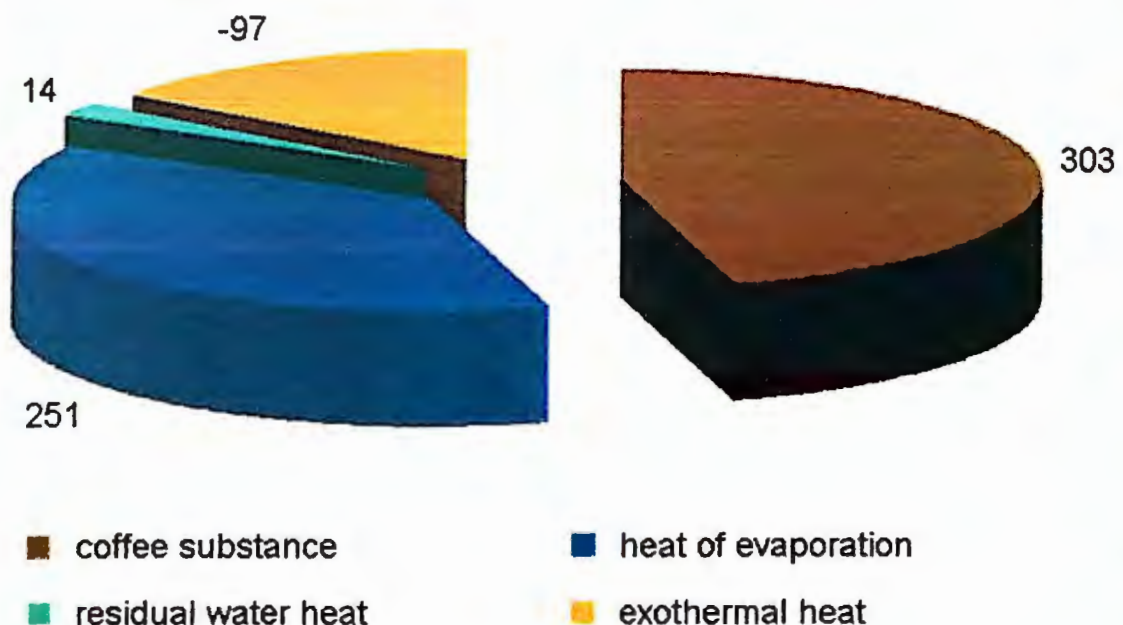


Fig. 7: Heat energy for coffee roasting in kJ/kg green coffee

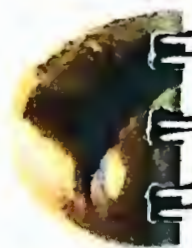


The specific heat energy requirement comprises the required water evaporation energy, the energy for heating the residual water and the heat energy for heating the dry coffee substance. Of course the released exothermal heat reduces the calculated energy for the roasting process.

In the above example (Fig. 7), the greatest share of the heat energy requirement is needed for evaporating the water present in the green coffee. This share can change depending on coffee moisture and roasting degree. At higher levels of green coffee moisture, the share of water to be evaporated is greater and inevitably also the requisite heat energy requirement.

# 6 PHYSICAL CHANGES

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## 6.1 GENERAL INFORMATION

Unlike the chemical changes, the physical changes in the coffee beans during the roasting process with respect to color, volumes, form and loss of water and weight are easily recognizable and easy to measure.

As a result of the roasting process, the major share of the water present in the green coffee evaporates, the coffee beans expand and the color of the beans changes. The thin surface skin of the bean loosens itself from the coffee bean.

The loss of water and expansion of volume in the coffee bean give the cellular tissue a dry and brittle texture. This eases the crushing of the coffee beans and increases the extraction capability.



## 6.2 FORM/STRUCTURE

The form of the coffee bean generally resembles a semi-ellipsoid (Fig. 8).

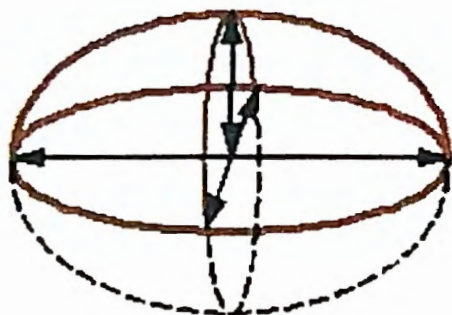


Fig. 8: Semi-ellipsoid;  
shape of a coffee bean

Compared to Arabica beans, the Robusta beans, when looking at the flat side of the bean, are somewhat rounder. Pearl beans have a geometry that corresponds more to a full ellipsoid. Pearl beans originate from single-seed cherries. A statement about the sort based on bean size is not possible. Even large-bean Robustas are being offered at present.

## 6 PHYSICAL CHANGES

A cross-section of the longitudinal axis reveals the special structure of a coffee bean (Fig. 9).

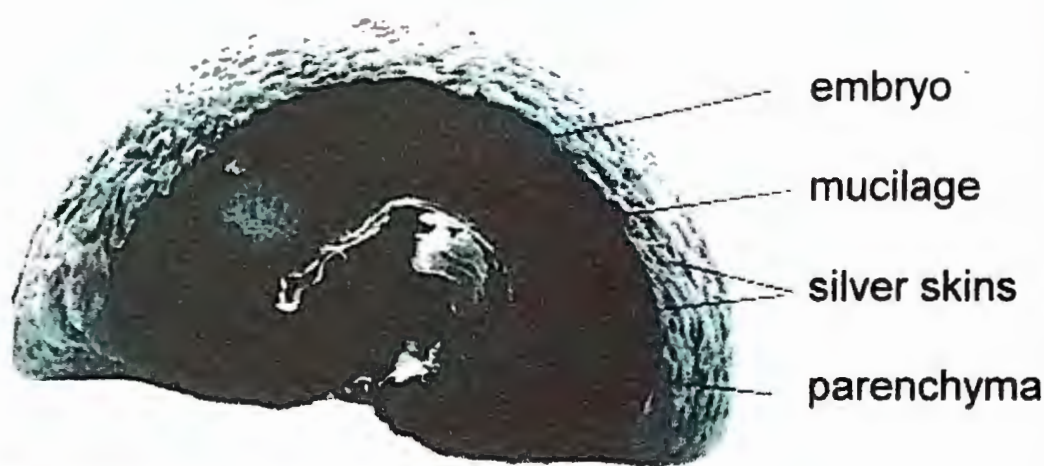


Fig. 9: Green coffee bean, Brazil

The cotyledonal tissue with the embryo in the middle is rolled up like a balled fist. Because of this, a part of the bean surface lies in the so-called "shadow area" and has no direct possibility of contact. The notch represents an open connection on the flat side of the coffee bean.

In highland coffees, the notch is closed and the inner bean structure firmer than in coffees growing in lower-lying regions. Highland coffees inevitably have greater density.

The strip of tissue originating from the embryo is two-ply and is separated by the "mucilage", a viscous layer. In the green coffee state both layers lie close together. The space between these two layers can increase through a heightened build-up of pressure during roasting.

The silver skin found on the outer surface of the coffee bean is clearly recognizable. It lies firmly on the cellular tissue. The silver skin found in the bean notch does not form such a firm connection with the cellular tissue. The more or less loose skin is held by the curved form of the notch.

The tissue of the coffee bean (parenchyma) is composed of many cells. A microscopic imaging of a piece of a coffee bean (Fig. 10) shows the complex cell structure with the many hollow cavities.

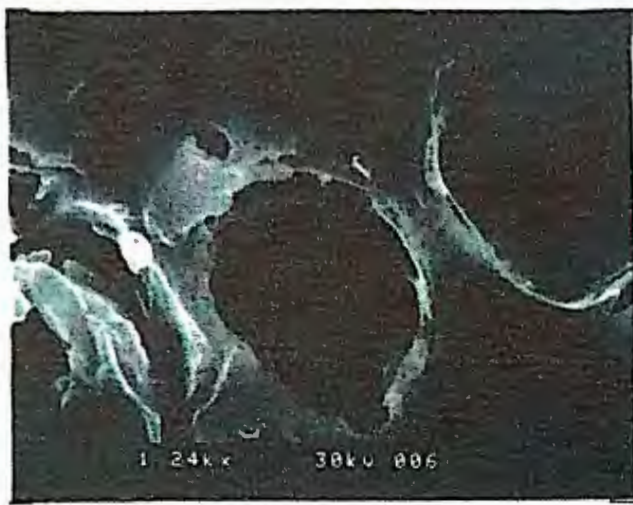


**Fig. 10:** Cells, scanning electron microscope

The cell core is enclosed in a thin, semi-permeable cellular membrane and bordered by a solid, cellulose-like cell wall. The cytoplasm surrounding the core contains in essence the substances already named in the “Green coffee” section. The more compact cell structure is clearly visible at the outer edge of the coffee bean.

## 6 PHYSICAL CHANGES

The enlargement (Fig. 11) done by a scanning electron microscope affords a look into the cells of a coffee bean. A single Arabica coffee bean is incidentally composed of approximately 1 million single cells. Each one of these cells makes its contribution to the end results.



**Fig. 11:** Cells, scanning electron microscope

The form of the coffee bean does not change substantially when roasted. The expansion of volume when roasting causes the round side of the coffee bean to arch through the longitudinal expansion and enlarge the notch. In highland coffees, the drawn-in notch opens less quickly during roasting and altogether less than coffees from lower-lying regions.

In green coffee beans, the surface on the notched side is generally somewhat drawn-in. Because of the pressure build-up in the cells during roasting, these surfaces form more of a level surface.

During roasting and through the formation of steam and gas (mainly carbon dioxide), there is a high build-up of pressure inside the cells. The cell volumes expand. Due to the expansion of the cell peripheries, the cell walls become thinner and the micropores larger. Moreover the periphery has become more brittle through the loss of water. Inside the cell, an equilibrium develops between the built-up pressure and the permeability of the cell structure.

If the pressure inside the cells has become too great, the gas mixture seeks an escape route at the weakest spots of the coffee bean. At a specific roasting degree, an audible cracking can be noticed. In the area of the weak spot, sections of bean are sometimes abruptly blown off, giving rise to the typical cracking sound. These weakest spots are generally found on the flat side of the coffee bean. Hairline cracks form in this area. If the pressure is particularly high, the hairline cracks can widen and become visible. These cracks are found particularly at the notch of the bean and on the lateral edge (Fig. 12).



Fig. 12: Roasted coffee bean with cracks

Further along in the course of roasting, a second cracking occurrence can come about, especially for dark roasting degrees. The first audible cracking is caused for the most part by the escape of steam, the second cracking, however, is caused mainly through the formation of carbon dioxide.

## 6 PHYSICAL CHANGES

### 6.3 COLOR

The color changes during roasting depending on the coffee sorts and possible pretreatment. For coffees from high-altitude areas of cultivation, the color change sequence runs from tender green to yellow, yellow-brown, light brown, dark brown to black-brown. Coffees that grow in the lowlands first become pale, quasi-colorless, before getting the yellow hue. The change of color from tender green to yellow in highland coffees and the paling in lowland coffees is a change toward a lighter appearance.

Yellowing starts at approx. 130°C. From this phase on, a gradual change from light to dark takes place. In the range from yellow to light brown, the bean surface can have an uneven and speckled appearance, especially in coffees grown in the lowlands. In the further course of roasting, this evens itself out again and the surface of such beans takes on a regular appearance.

The color of the roasted coffee is an indication of the roasting degree and can help the operator to manage and control the process. The roasting degree is an extremely important criterion for the quality of the coffee. Coffee producers set a very specific roasting degree for every product offered on the market. The roasting degree is worked out based on market research, many years of experience and intensive sensory tests.

The color of the bean surface alone, although useful as a reference parameter for roasting, does not allow a clear statement to be made about the roasting degree as a whole. Different temperatures inside the coffee beans can result in a uniform and thorough roasting not having taken place. Especially for very short roasting times, it can be expected that the color in the core of the bean will remain lighter than the bean's surface. Moreover, a shiny coffee bean surface caused by escaping oil can affect the color assessment.

For this reason, the relationship between roasting degree on the one hand and color value on the other hand is only meaningful by assessment of the coffee in a ground state.

There is no standard, i.e. standardized measurement procedure, for determining the color of roasted coffee. Terms such as "light", "medium", "dark", etc., although they enable a rough classification of roasting degrees, are insufficient for making qualitative and economical statements, i.e. assessments.

The roasting degrees and color values dealt with in this chapter all refer to results measured with the color-measuring instrument model Colorette 3a made by PROBAT-WERKE, D-Emmerich. The table below enables proper utilization of these scale values. For this, the terms in the SCAA Roast Designation are compared with the measurement values of the Colorette 3a. The color values refer to ground coffee subsequent to the internal Probat-standardized sample treatment.

<b>SCAA</b>	<b>PROBAT-WERKE</b>
<b>Roast Designation</b>	<b>Colorette 3a</b>
<b>very light</b>	<b>140</b>
<b>light</b>	<b>120</b>
<b>mod. light</b>	<b>110</b>
<b>light medium</b>	<b>95</b>
<b>medium</b>	<b>80</b>
<b>mod. dark</b>	<b>70</b>
<b>dark</b>	<b>55</b>
<b>very dark</b>	<b>45</b>

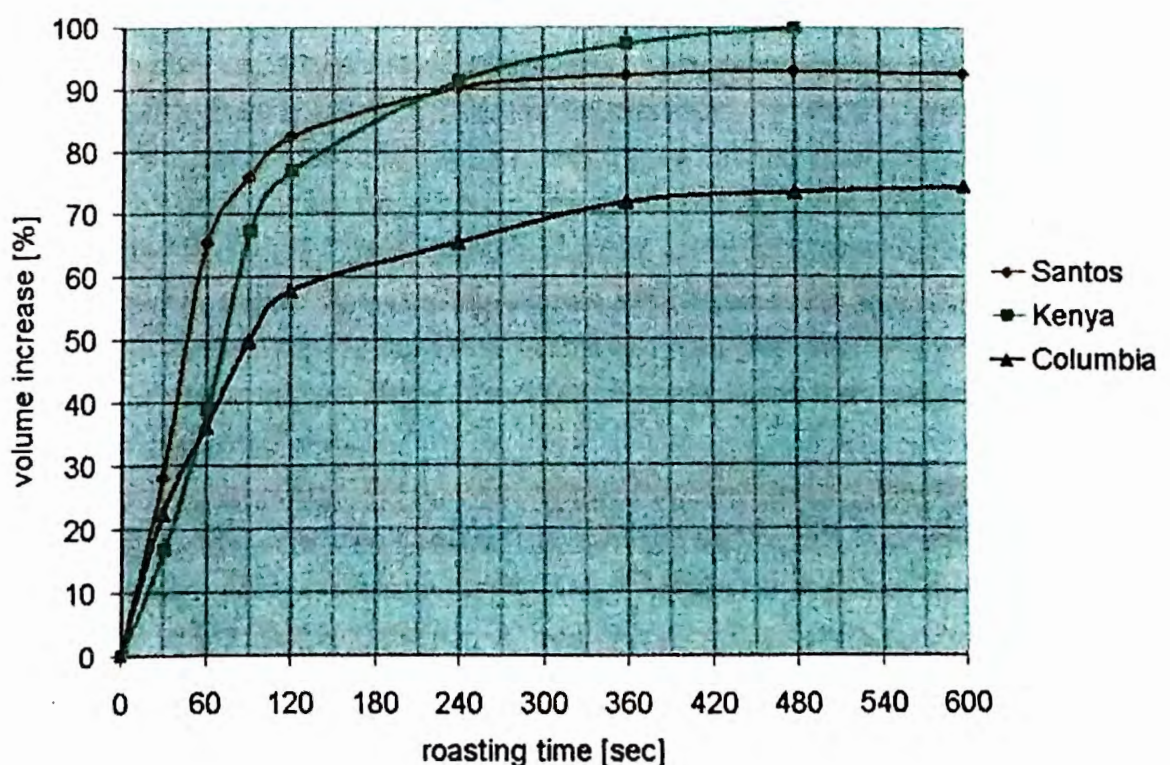
# 6 PHYSICAL CHANGES

## 6.4 VOLUME

The volume of the coffee bean expands during roasting. As a result, the dimensions of the bean change more or less proportionally in length, width and height. Through the formation of steam and gas, there is a high build-up of pressure inside the cells of the beans causing the coffee beans to swell. The permeability of the cell periphery, i.e. the porosity, is not sufficient to allow the quantity of steam and gas to escape completely before the pressure builds up. The bean structure, the green coffee moisture and the coffee temperature profile during roasting have a decisive influence on the expansion of the beans. Depending on the coffee sort, roasting time and roasting degree, the increase in volume can more than double.

The course of volume change is also sort-related. So-called "hard" coffees such as Kenya coffee, offer as it were more resistance, which causes the volume to increase more slowly at the start of roasting compared with "soft" coffees.

The figure (Fig. 13) shows the proportional volume increase in coffee beans for Santos, Kenya and Columbia coffee sorts during roasting.



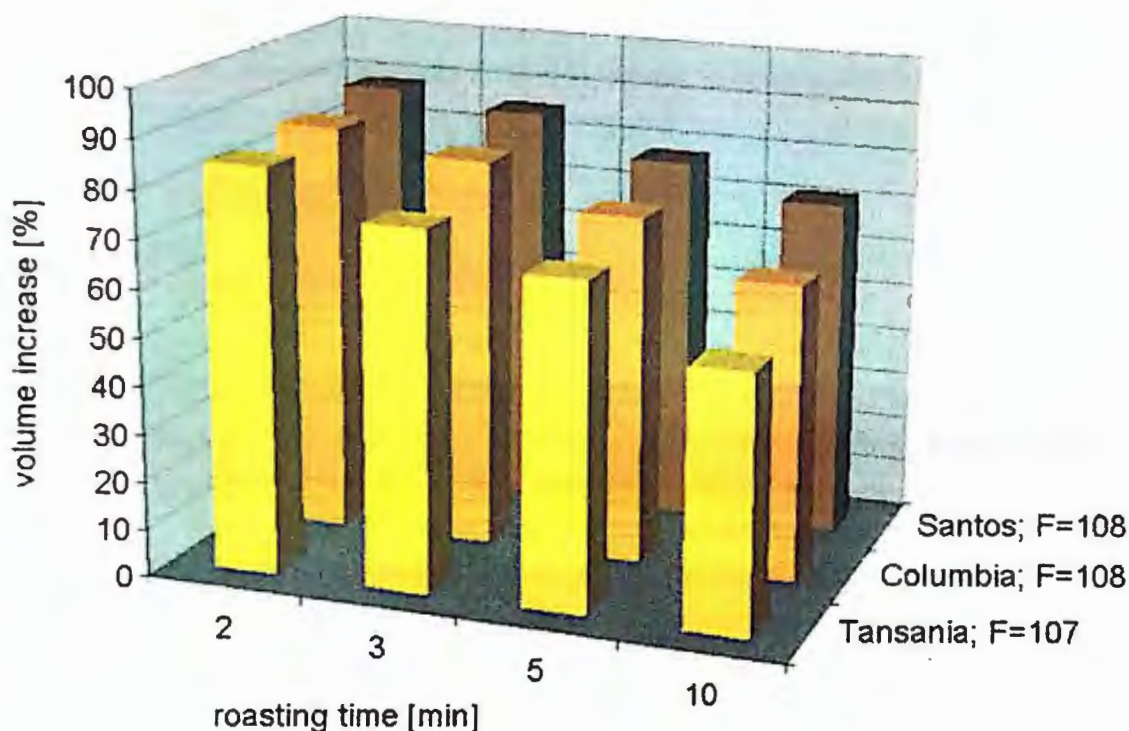


Fig. 14: Expansion of coffee beans

The influence of the roasting time on the volume of the roasted coffee beans becomes apparent from a further figure (Fig. 14). The volume of a Santos coffee roasted in a roasting time of two minutes at a roasting degree of 108 scale degrees expands by around 89%. The volume of the same coffee sort roasted at the same roasting degree but for a longer roasting time of 10 minutes increases by approx. 72%. There is a tendency in all coffee sorts towards a decrease in volume for extended roasting times and an increase in volume for shortened roasting times. Absolute volume values and absolute influence variables on volume expansion brought about by changes in the roasting time depend heavily on the sort.

The volume of a green coffee bean with a length of 8.6 mm, a width of 6.7 mm and a height of 4 mm is calculated to be 120 mm<sup>3</sup>. The individual dimensions after roasting expanded to a length of 10.5 mm, a width of 8 mm and a height of 5 mm. The roasted bean volume now amounts to some 220 mm<sup>3</sup>, which means a volume increase of 83%.

## 6 PHYSICAL CHANGES

The expansion in volume causes the silver skins on the external surface of the beans to loosen. The difference in expansion between bean surface and skin causes tension, whereby the skins tear and flake off.

### EXCURSUS:

To delve more deeply into the subject of "volume expansion", it would do well to take a look at a special aspect: the "glass transition temperature". What is described is the consistency of the coffee bean and the concomitant condition under which it can expand with greater ease or difficulty. For this, the parameters for the "temperature" of the coffee bean and those for its "water content" are placed in a relationship.

Depending on the coffee temperature and moisture content of the coffee beans, they are either in a glass-like (hard) condition or one that is rubber-like (leathery). The transition from a glass-like to the rubber-like state is defined as "glass transition temperature". For a bean water content of 12% for instance, the transition from glass-like to rubber-like is reached at approx. 100°C. For a water content of 4%, the transition temperature lies at approx. 140°C. If during the roasting process, for example, the coffee beans with this water content exhibit a temperature of 150°C, the glass transition temperature curve is exceeded and the beans will be in a rubber-like condition.

To enable portrayal of the water content in the following figure (Fig. 15), the water content value was raised 10-fold.

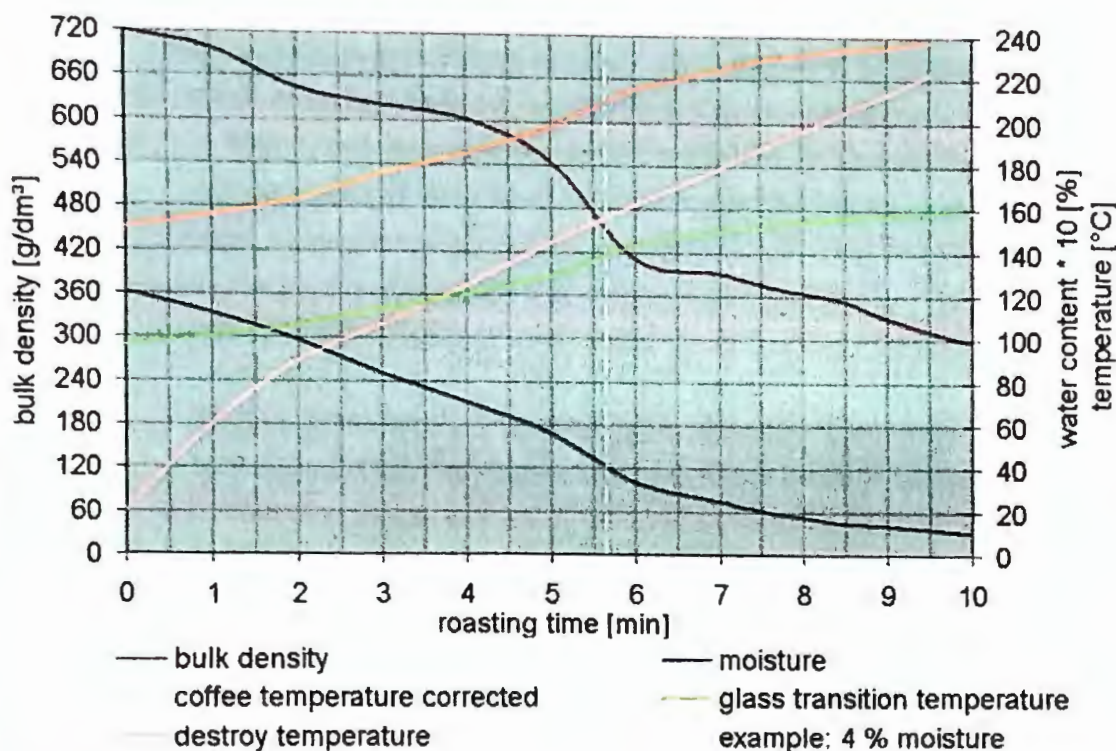


Fig. 15: Roasting sequence (bulk density/glass transition; coffee sort: Columbia)

As can be clearly seen in the figure (Fig. 15), the essential volume expansion of the coffee beans starts once the glass transition temperature has been exceeded. The volume expansion results from the sinking value of the bulk density. This relationship is explained in Chapter 6.6 "Density". In the range above the glass transition temperature, expansion is facilitated by the leathery state of the product. The coffee beans are thereby less sensitive to breakage further along in the roasting procedure. The glass transition temperature is not undershot until the cooling procedure, and the hard state of the beans is restored.

Breakage or cell destruction can come about if the temperature is too high. Just like the glass transition temperature, the course of the destruction temperature is dependent on the moisture of the roasted coffee. To reiterate, for a residual moisture content of 4% in the coffee, the glass transition curve is overshot at a temperature of 140°C. As the roasting procedure proceeds, i.e. as the coffee temperature rises, the coffee temperature and destruction tem-

## 6 PHYSICAL CHANGES

perature approach one another. Cell destruction cannot be ruled out for very dark roasting degrees, particularly on the surface.

This relationship is portrayed in the figure above (Fig. 15). The values cited can be read off from the light-blue, dashed, vertical auxiliary line (4% moisture, i.e. scale value 40).

### 6.5 WEIGHT LOSS

Weight loss during roasting, also known as substance loss, is inseparably associated with the water content of the green coffee, with the physical and chemical changes in the coffee and with the waste-gas behavior. The total loss of weight can fluctuate between 12% and 23%.

The decrease in bean weight during roasting is made up of the loss of water ( $H_2O$ ) and skin as well as dry substance, which occurs in the form of carbon dioxide ( $CO_2$ ), carbon monoxide ( $CO$ ), nitrogen ( $N_2$ ), volatile acids and volatile aromatic compounds ( $CH$ ). Water loss makes up the greatest proportion of weight loss. The original green coffee moisture considerably influences substance loss during the roasting process. Related to the dry substance, the loss of carbon dioxide compared with all other compounds is by far the greatest (see Fig. 16).

Foreign particles, tiny stones in particular, which were not removed in advance by the green coffee cleansing, can naturally affect the results of substance loss. As a rule these foreign particles are separated out of the coffee immediately after the roasting and cooling process. The larger and lighter roasted coffee beans afford an excellent opportunity for separating the remaining stones from the coffee. If the green coffee was effectively cleansed, the part by weight is very low. Nonetheless, in unfavorable cases up to 0.2% stones or similar foreign particles were removed from the roasted coffee of certain Robusta sorts.

The total weight loss during roasting lies, for example, for a specific Arabica coffee with a roasting degree of 110 scale graduation (Colorette 3a) at approx. 15.1%. A darker roasting degree of 80 scale graduation raises the substance loss to approx. 17.3%. The figures for substance loss when processing Robusta coffee sorts are as a rule higher than those for Arabica coffees of equivalent color. Shown in the following figure (Fig. 16) is the roasting-related loss trend for different green coffee sorts and two different roasting degrees, respectively.

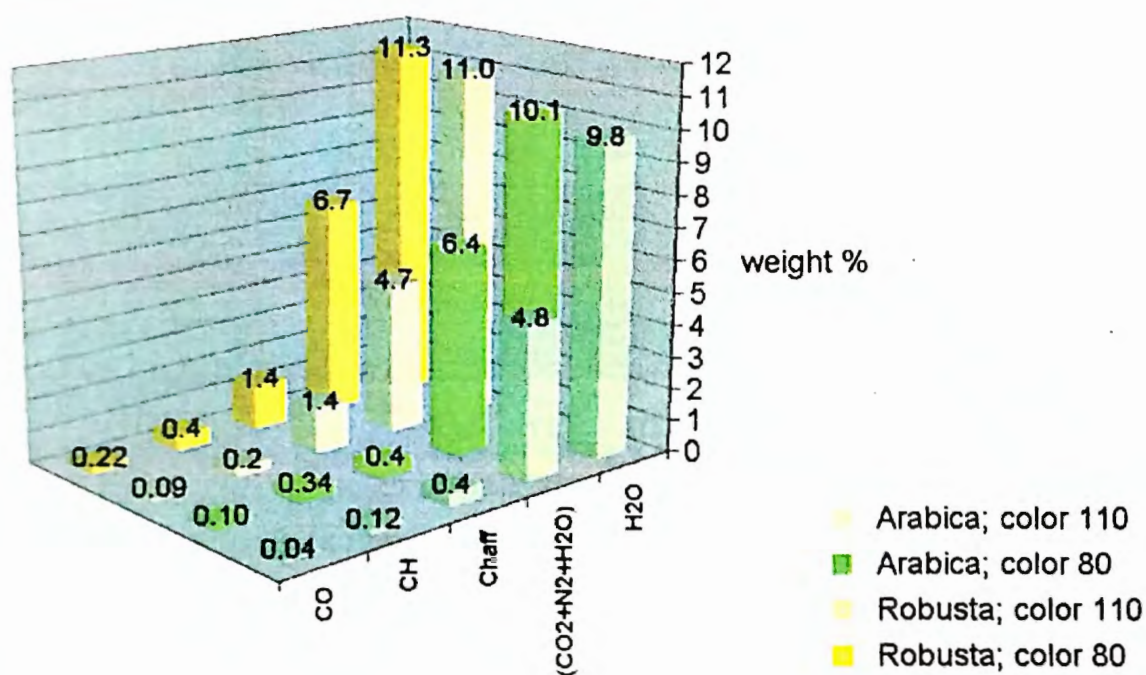


Fig. 16: Loss of substance

## 6 PHYSICAL CHANGES

The roasting degree is decisive in limiting the roasted yield, i.e. the loss of dry substance. The connection between loss of dry substance and roasting degree, shown for three different green coffee sorts at a roasting time of approx. 8 minutes, is demonstrated in the following figure (Fig. 17).

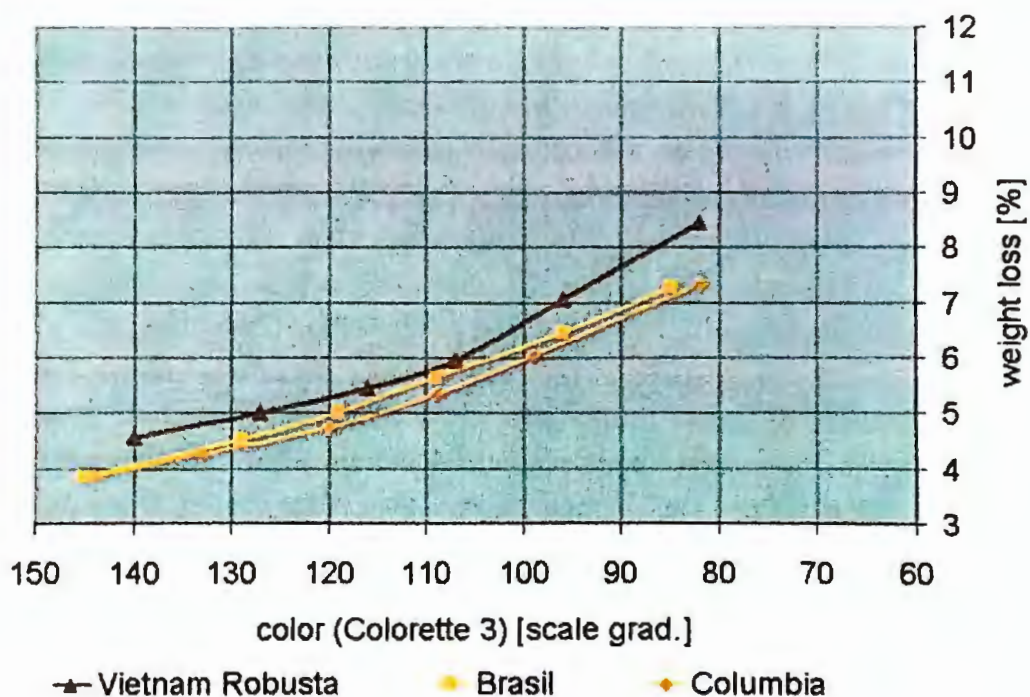



Fig. 17: Loss of dry substance during roasting (roasting time approx. 8 min.)



The proportional loss of dry substance relates to the dry green coffee goods and the dry roasted coffee goods, i.e. the water contents have been subtracted. Loss of skin is not included in the substance loss.

Skin loss pertains mainly to the silver skins found on the outside surface of the bean. Depending on the green coffee sort and the quality, a greater or lesser quantity of skin is to be expected. Washed Arabica coffees, for example, have a smaller proportion of skin than unwashed coffees. The proportion of skin determined for untreated Arabica coffees runs from 0.3% to 0.9% and for Robusta coffees, proportions of up to 2% are common. The greatest proportion of skin by far, 90 – 95%, loosens itself from the surface of the bean during roasting and is discharged along with the outgoing air.

Unlike the surface skins, the silver skins found in the notch of the entire bean are not released until grinding. This proportion of skin generally remains in the ground coffee product.

In the coffee processing industry, water quenching is implemented to abruptly stop the roasting sequence once a specific coffee temperature or coffee hue has been attained. This ensures that reproducible roasting degrees are achieved from charge to charge. By specifying this water charge quantity, an almost infinitely variable increase of from 0.5% to 5% water content in the roasted coffee can be achieved. The yield, i.e. the weight loss, will automatically be positively influenced thereby. The effect of the water content on the quality of the roasted coffee, however, should not be underestimated, particularly in connection with the shelf life of the coffee.

Owing to the high gas pressure in the cells of the coffee bean, gas is constantly released until pressure equalization with the surroundings comes about. The gas in this instance is chiefly carbon dioxide. This gas-release behavior results in weight loss. Different degrees of loss can be expected according to coffee sort, roasting degree and roasting time. The average total gas-release amount is approx. 0.8%. After a dwell or storage time of 2 hours, loss of weight can already amount to 0.05%, and after 8 hours approx. 0.1%.

# 6 PHYSICAL CHANGES

## 6.6 DENSITY

The loss of mass and expansion in volume during roasting result in a reduction in the density of the coffee bean. Important for warehousing and packing is the bulk density of the coffee. The bulk density is the mass in g that occupies a volume of 1 dm<sup>3</sup> or, accordingly, the mass in kg for a volume of 1 m<sup>3</sup>.

The reduction in bulk density during roasting is shown in the following diagram (Fig. 18).

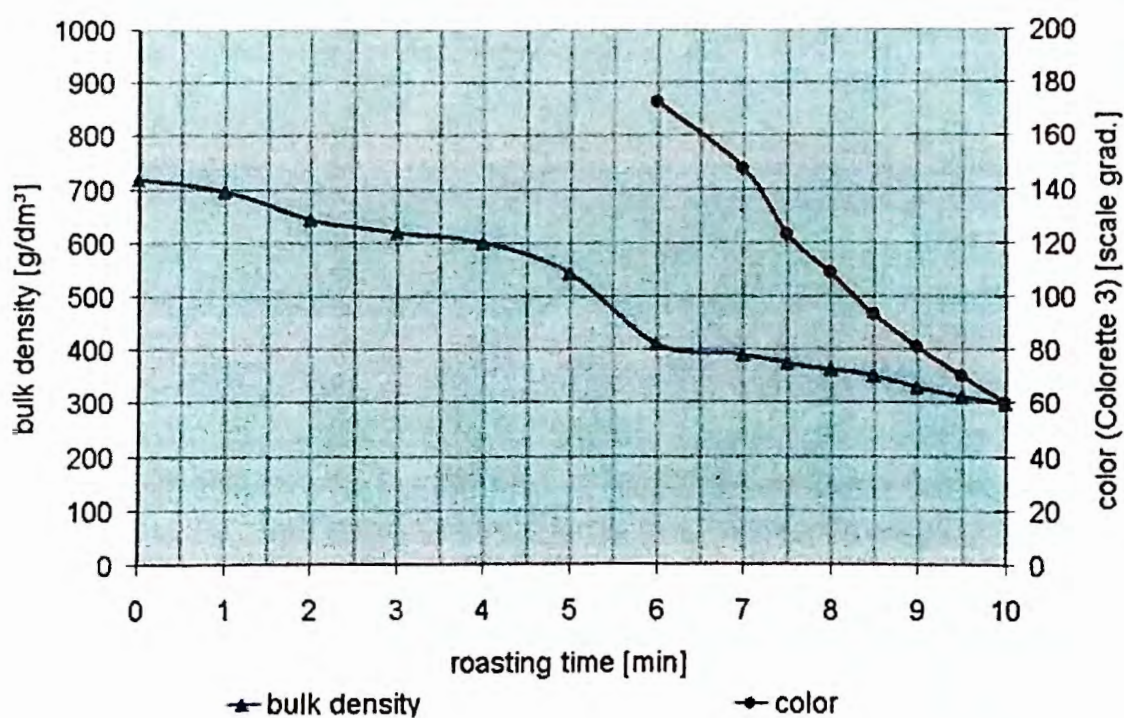


Fig. 18: Development of bulk density during roasting (coffee sort: Columbia)

Owing to the loss of mass, the high short-term loss of water in the roasting time range between the 5th and the 6th minute is automatically mirrored in the bulk density. The course of the residual water and that of the bulk density is practically identical. Water loss evaporation on the one hand, and the volume increase on the other hand run simultaneously.

Volume expansion during the roasting procedure has an effect on the bulk density of the roasted coffee beans. Shown in the bar chart (Fig. 19) exemplifying the Columbia coffee sort are the bulk densities determined for coffees produced in roasting times of 3 minutes, 5 minutes and 10 minutes. The 10-minute roasting time resulted in a bulk density of  $382 \text{ g/dm}^3$ , hence a change in density of some 7%. The change of roasting time from 10 minutes to 3 minutes resulted in a bulk density reduction of approx. 12%.

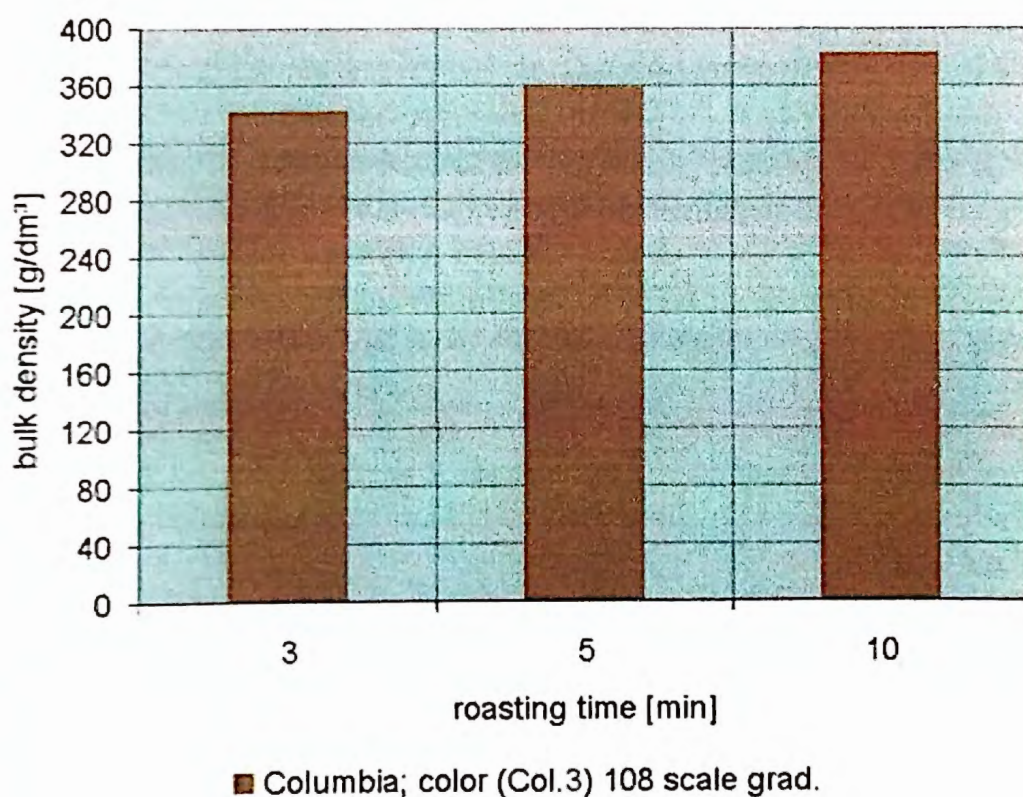


Fig. 19: Roasting time/bulk density; coffee sort: Columbia

# 6 PHYSICAL CHANGES


## 6.7 DEHYDROLYSIS

The removal of water is called “dehydration”. Dehydration progresses in two stages during roasting. Up to a temperature of approx. 100°C, evaporation takes place, and subsequently vaporization.

Evaporation, i.e. vaporization is the term denoting the transition of a substance from a fluid or solid state to a gaseous state. In the roasting process, the vaporization of water is important for the economic efficiency and for the quality of the roasted coffee. Yield, i.e. substance loss, energy requirement as well as the course of the physical and chemical processes are influenced by the original quantity of water in the green coffee, i.e. the water content converted into steam.

The water content has a substantial influence on the behavior of the coffee beans during roasting. Thermal conduction in moister coffees, for instance, is higher than in dryer coffees. As a rule, green coffee has an approximate initial moisture concentration of 8% to 13% before roasting. The post-roasting water concentration in the roasted coffee beans lies between 0.5% and 3.5% dependent on coffee sort, roasting time and roasting degree. The influence of a possible water quenching at the end of the process is not taken into consideration here.

The transition from the fluid to the gaseous state progresses – as already mentioned – in two stages during the roasting process: evaporation and vaporization.



Up to a coffee temperature of 100°C the free water on the surface of the coffee beans is absorbed by the ambient air, which as a rule is the roasting air. Because of the relatively high temperature, the roasting air is able to absorb a great quantity of steam. The air velocity contributes to this evaporation process. A process takes place inside the bean to bring the moisture into equilibrium whereby there is a movement of water from the core towards the surface of the bean.

Once the boiling point of 100°C is reached, vaporization sets in. To be taken into account here is that the steam which forms simultaneously requires more space than the water did in its previous fluid state. The pressure in the cells begins to rise. The steam presses not only against the inner periphery of the cells but also against the surface of the water as well. This increase in pressure suppresses the boiling of the water. The continued feed of heat first of all raises the water temperature and thus the steam pressure inside the water until the latter becomes greater than the steam pressure acting upon the surface of the water. The water now boils, water vaporizes, the steam pressure above the water rises, etc.

Although steam continuously dissipates through the semi-permeable cell wall, it is still not enough to prevent a gradual rise in pressure. A pressure rise of, for example, about 1 bar raises the boiling point of the water from 100°C to 120°C, an overpressure of 4 bar raises the boiling point to 150°C. At this temperature and this pressure, the water is still in a fluid state. The pressure that has built up in the cells of the coffee beans in the end phase of the roasting process lies in an overpressure range of some 5 bar to 20 bar dependent on coffee sort, roasting time and roasting degree. An overpressure of 20 bar comes about in extremely dark coffee roasted in a short time.

## 6 PHYSICAL CHANGES

The influence of the inner pressure on water vaporization takes place particularly in the second vaporization phase. During this time, the increase in volume is also inevitably highest.

Besides being dependent on the temperatures, the reactions taking place during roasting are also dependent on the prevailing pressures. Because of this, the water quantity on hand in the green coffee not only has an influence on the transition of heat but also on the course of many individual reactions.

An example of the change in the water concentration of coffee during roasting is portrayed in the following figure (Fig. 20). The data refer to a Columbia coffee with an initial water concentration of approx. 12%. The coffee was roasted "light" in 7.5 minutes and "dark" in 9 minutes.

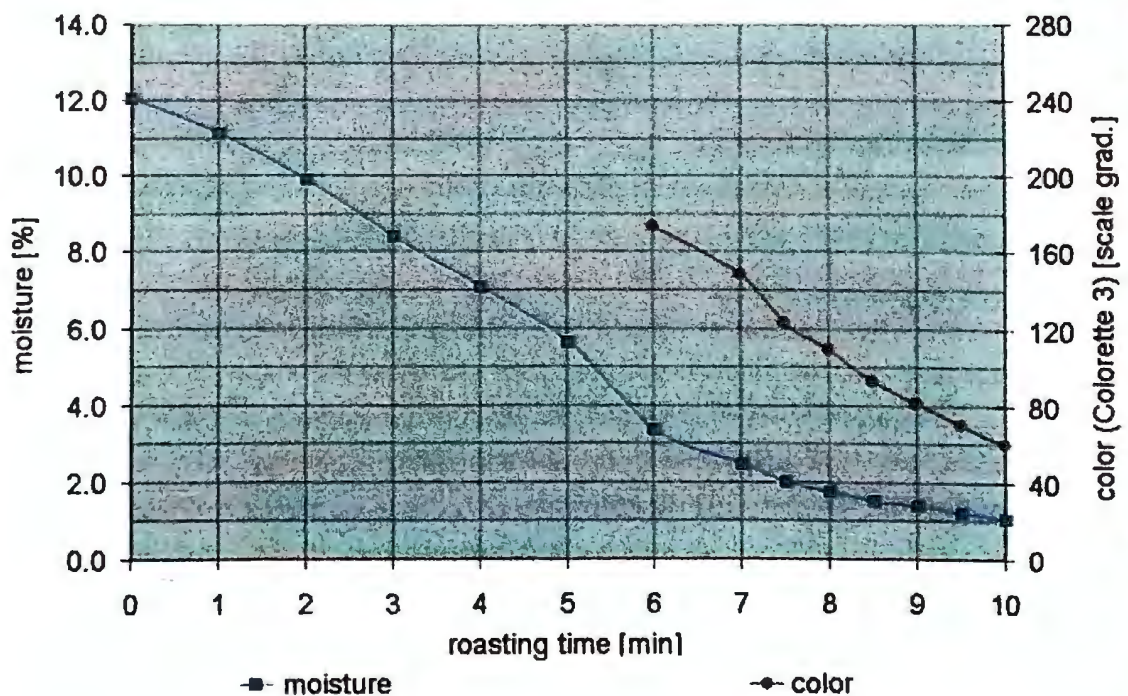


Fig. 20: Development of moisture during roasting

Water loss begins immediately at the start of roasting. In the first roasting phase, i.e. up to a temperature of  $100^{\circ}\text{C}$ , the loss of water occurs through evaporation of the water at the surface of the coffee beans. In this phase, i.e. during the first 1.5 minutes, the water loss progresses in a relatively flat curve. All in all, 1.4% water evaporates here. The specific water loss is then approx. 0.9% per minute.

In the second roasting phase, the temperature is above  $100^{\circ}\text{C}$ . Due to the vaporization, the loss curve now has a steeper gradient. A further 1.4% water per minute is vaporized. After 5 minutes (from the start of roasting), more than half of the water initially on hand has vaporized.

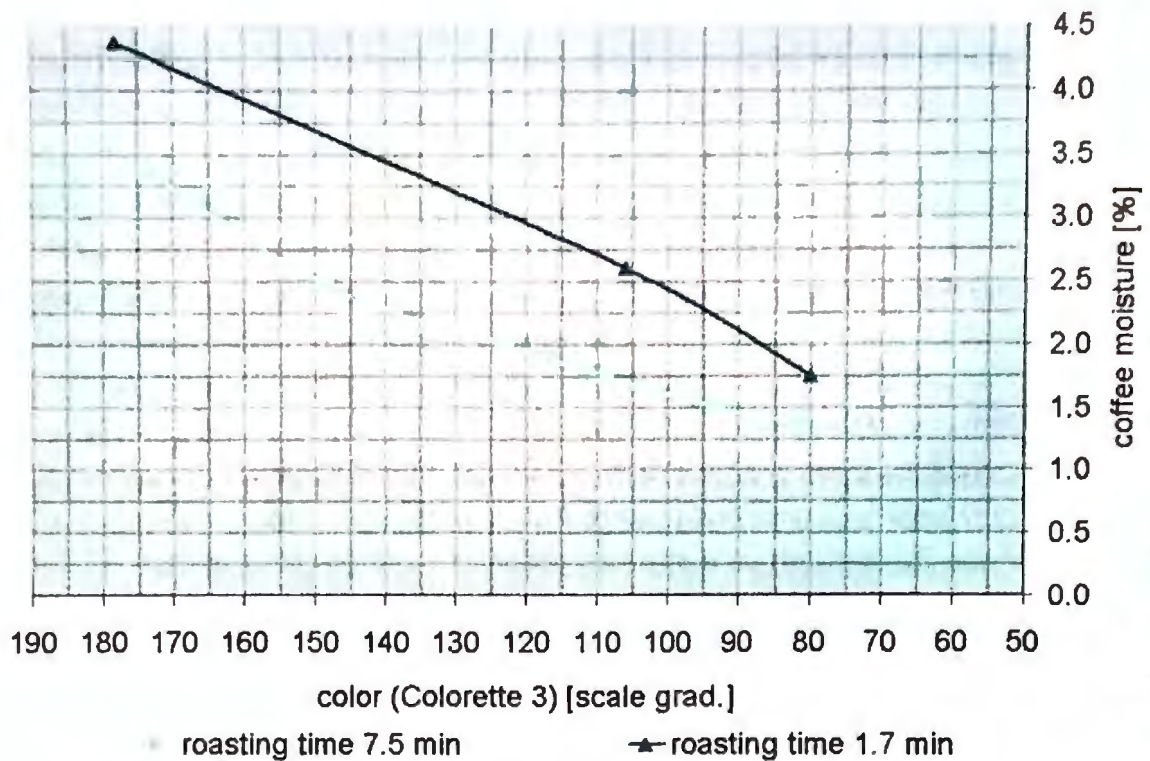
The third phase, i.e. between the 5th and 6th minute, can be clearly and visibly discerned. Seen in terms of time, water loss is greatest in this phase. At 2.3% per minute, vaporization is almost twice the previous rate.

The low water loss of 0.9% at the start of roasting is explained by the fact that the boiling point of water has not yet been reached. Through evaporation on the surface of the coffee bean, less water is given off.

The heavy vaporization in the third phase, i.e. in the 5th and 6th minute of roasting, can be attributed to the volume increase in the beans and to the fact that the pressure-related tensions have given rise to cracks at some of the cell peripheries. At times, this is even visible on the surface of the beans. As a result of crack formation, the internal pressure sinks and water vaporization is accelerated.

In the further course of roasting, after approximately 6.5 minutes, due to a continued pressure rise caused by additionally released gases, there is less water loss. To be taken into account is that less quantities of water arise in this exothermal phase due to oxidation. For this reason an exact statement on the steam quantity is not possible. The water quantity released by oxidation of up to 1%, related to green coffee can be approximately calculated from the exothermal energy. Cited in the dissertation of Raphael Geiger (ETH No. 15430; CH-Zürich 2004) is a chemical-reaction-related water content release of up to 4%.

## 6 PHYSICAL CHANGES



**Fig. 21:** Residual moisture development dependent on roasting degree

The residual water quantity in the roasted coffee is for the most part on hand as fixed water. The free water is for the most part vaporized. The residual water quantity depends heavily on the roasting degree and roasting time. The darker the coffee has been roasted, the less water is left over. At shorter roasting times, less water is vaporized, whereby more residual water remains in the roasted coffee compared with longer roasting times.

Shown in the diagram (Fig. 21) are the roasting-degree-related residual water quantities in roasted coffee for a medium roasting time of 7.5 minutes and a very short roasting time of 1.7 minutes.

For a color value of 120 scale graduation (light roast), the roasting-time-related residual water content lies approximately between 2% and 3%. For a medium roast coffee, a residual water quantity of approx. 1.4% to 1.8% remains.



## 6.8 OIL MIGRATION

The major portion of the lipids already on hand in the green coffee, i.e. the non-volatile fats and oils, is not changed in terms of quantity in the course of roasting. The greatest share of lipids by far is present in fluid form inside the cells. A portion of the enclosed lipid migrates, aided by the movement of gas, toward the surface of the coffee bean. Escape is prevented or at least retarded by the dense structure of the cellular tissue in the area of the bean surface.

For certain types of roasting, especially for short roasting times and dark roasting degrees, the sporadic escape of liquid fat particles cannot be prevented. Isolated, fine drops of fat then form on the surface of the bean after roasting. This phenomenon is known as "sweating coffee".

In extreme cases, if the coffee is roasted very darkly in an extremely short time, oil drops already emerge from the bean during roasting. As a result of the movement and mutual contact of the coffee beans, an even film of oil is formed on the surfaces.

In all probability, the internal pressure in the cells and the concomitant speed of gas desorption is the driving force behind oil migration. Also playing a role here are the structure of the tissue, the porosity of the beans, the viscosity of the oil and the ambient atmosphere of the coffee beans.

A coffee bean surface fat content of from 1.5 to 2 weight percent has been measured for dark-roast coffees.

# 7 CHEMICAL REACTIONS

## 7.1 GENERAL INFORMATION

During the roasting process, many complex reactions take place which give the coffee its color, its taste and its typical coffee aroma. The Maillard reaction as well as pyrolysis, hydrolysis and oxidation all play an extraordinarily important role in this regard. Almost 1000 different components are formed out of just a few initial compounds. Almost 850 different volatile aromatic components have been identified to date (Fig. 22). The major portion of these is made up of volatile aromatic compounds.

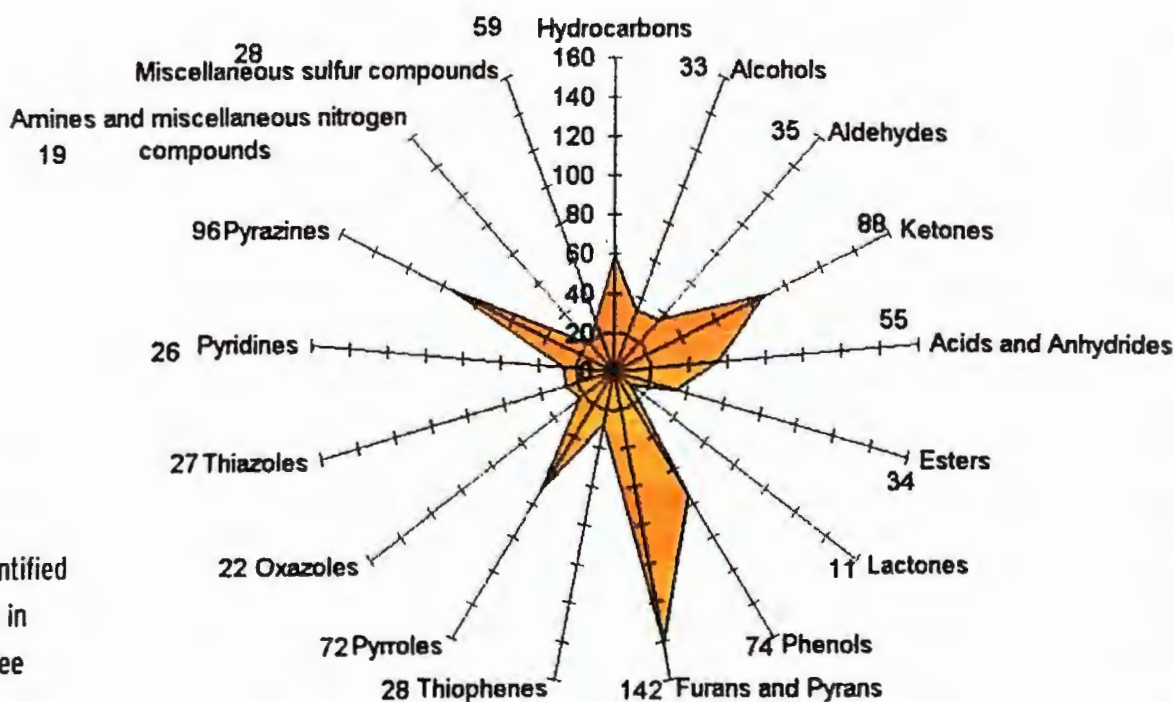


Fig. 22: Identified components in roasted coffee



In terms of quantity, the many different aromatic compounds make up only 0.1% in total of the roasted coffee weight. Despite this low mass, roasted coffee is one of the most aromatic of foodstuffs. Many of the aromatic components relevant for the coffee beverage are present in the ppm, i.e. ppb range or even only in traces. The low quantity, however, sometimes has an enormous influence on the quality.

Olfactory perception, i.e. olfactory intensity is not only dependent on the concentration, but also on the corresponding olfactory threshold. Only a few aromatic components are present in high concentrations with a low olfactory threshold. The olfactory threshold is the concentration of an aromatic compound at which recognition of the aroma is first possible. The components which are important for the coffee aroma are those whose concentrations in the coffee are higher than the olfactory threshold.

With a percentage in weight of approx. 38% to 45%, aromatic compounds of the furan group have the greatest proportion of volatile aromatic compounds. Pyrazines follow with approx. 25% to 30%. The share of pyridines is about 3% to 7% and pyrroles 2% to 3%.

Up to a coffee temperature of approx. 160°C, the course of the chemical reactions is endothermic, i.e. under thermal absorption. In a temperature range of 160°C to about 250°C, the transfer of heat is augmented due to exothermic reactions (pyrolysis). At a coffee temperature of around 220°C, the exothermic reaction is at its highest. The thermal energy being released is generally insufficient for continuing the roasting process in the desired profile without additional heat.

# 7 CHEMICAL REACTIONS

## 7.2 MAILLARD REACTION

Described by the "Maillard reaction" is a non-enzymatic browning process in which reducing sugars react with amino acids. This process was named after L.C. Maillard who did research in this area for the first time in 1912. The extremely complex chemical reaction described by Maillard provides important knowledge for the fields of foodstuff chemistry as well as physiology. For coffee roasting, the Maillard reaction is important particularly with respect to coloration and aroma.

Most of the aromatic compounds are formed by the Maillard reaction. The colorants, called melanoidins, arise from the non-enzymatic browning reaction.

The course of the Maillard reaction comprises many successive single reactions. In the first phase, the saccharides react with amino compounds, peptides or proteins from which reactive, multifunctional intermediate products develop.

Amadori products are produced from the glucosamines in the next stage through Amadori transposition. Arising from the intermediate products are, among other things, diketons, furanons, furans and pyranons.

Further along in the Maillard reaction, the compounds formed thus far react with amino compounds. This so-called "Strecker synthesis" describes the production of  $\alpha$ -amino acids through the action of sodium cyanide and ammonium chloride on aldehyde with subsequent hydrolysis. This connection was discovered in 1862 by Mr. A. Strecker, whose name became the eponym for the term. During Strecker synthesis, the dicarbonyl compounds, for example, react with amino acids. Strecker synthesis provides carbon dioxide, aldehydes and  $\alpha$ -aminoketones. Pyrazines come about through condensation.

The advanced stage of the Maillard reaction becomes evident through the formation of red-brown to black-brown melanoidins. These polymers of high molecular weight are very important for the characteristic coloration and the characteristic bitter taste profile.

The majority of the bitter-tasting compounds arise during the Maillard reaction. Substances composed of pyrrolin and sucrose have an intensely bitter taste.

In summary, the Maillard reaction and Strecker synthesis convert carbohydrates into compounds belonging to the ketone, furane, aldehyde and melanoidin class of substances. Here, amino acids give rise to ketones, furanes and sulfide compounds. A relatively minor share of protein is converted into ketones and furanes and thereby also contributes to the aromatic compounds.

The decomposition of the carbohydrates through the Maillard reaction is exemplified in the bar chart (Fig. 23).

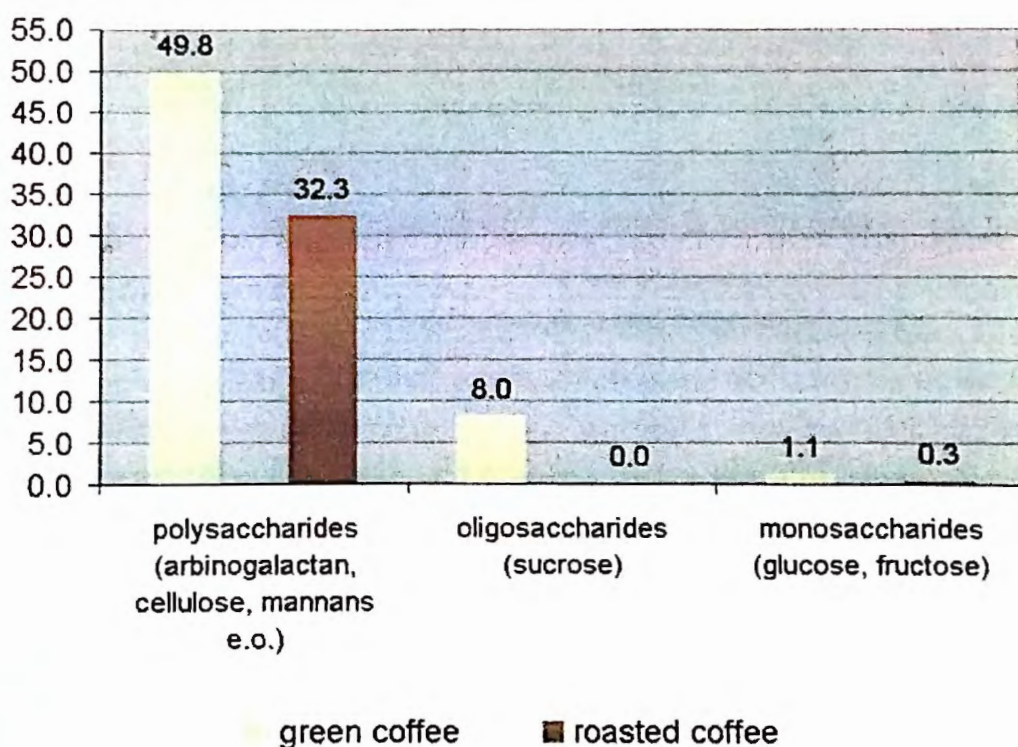
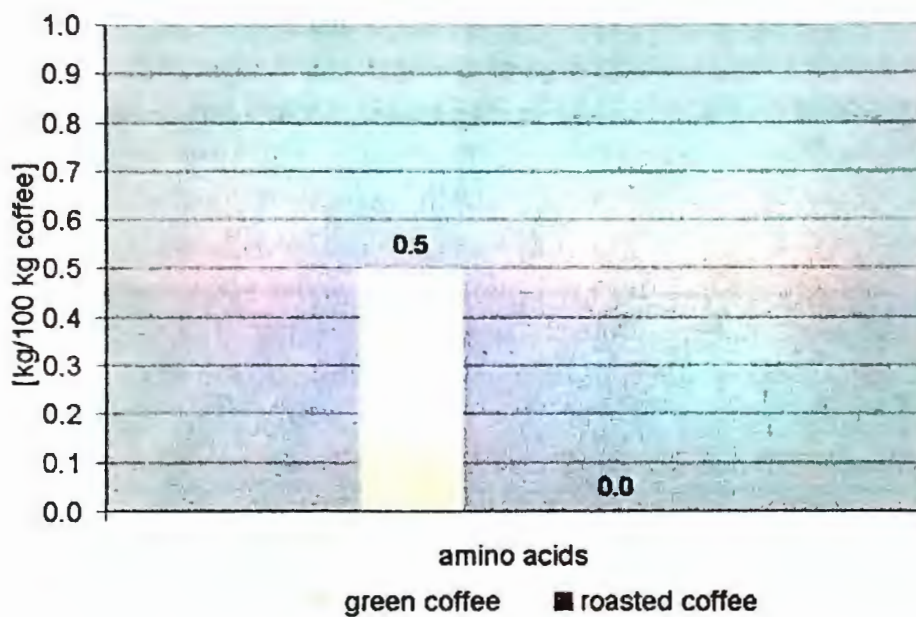


Fig. 23: Carbohydrate decomposition through the Maillard reaction

# 7 CHEMICAL REACTIONS

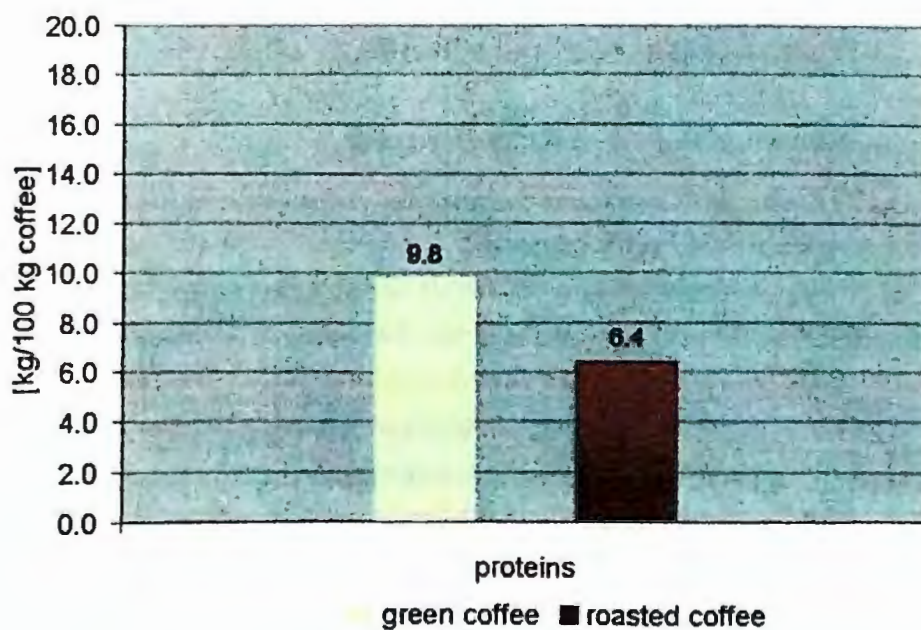
The amino acids originally present react completely with the simple sugars (Fig. 24).


**Fig. 24:** Amino acid decomposition through the Maillard reaction



As seen in Figure 25, only a minor share of proteins is decomposed.

**Fig. 25:** Protein decomposition through the Maillard reaction





The carbohydrates that have not broken down, especially the water-insoluble polysaccharides, make up the substance of the cell walls in roasted coffee. When the coffee beverage is made, most of it remains as coffee grounds.

### 7.3 PYROLYSIS

“Pyrolysis” describes the thermal decomposition of complex substances. During pyrolysis, single compounds of substances typical for coffee come into being as a result of decomposition. For instance, trigonelline gives rise mainly to pyridine. The decomposition of the chlorogenic acids leads to the phenols, while coffee oil gives rise to slight quantities of aldehydes and carbohydrates. During pyrolysis, carbon dioxide and carbon monoxide are released and water is formed.

The chlorogenic acids on hand in the green coffee are for the most part destroyed during roasting. Chlorogenic acid is partly responsible for the stimulating effect and bitter taste of coffee. Besides phenols, pyridines are also formed from chlorogenic acid. The relatively high concentration of phenols in Robusta coffees is due to the high chlorogenic acid content in the Robusta raw coffee.

The figure (Fig. 26) shows the decomposition of the chlorogenic acids. The apparent rise at the start of roasting is deceptive and is attributed to the general loss of substance occurring in this phase so that the proportional relationship of chlorogenic acid, related to the dry substance, increases for a short period. The absolute chlorogenic acid concentration, however, remains practically the same in this phase.

At a color value of 120 scale graduation (Colorette 3a), some 60% of the chlorogenic acids have decomposed and at 70 scale graduation approx. 90%. As a result, volatile aromatic compounds (phenols) are created. As a result of the decomposition products, the chlorogenic acids contribute to the development of taste and aroma. The decomposition products from chlorogenic acids taste sour and are in part considered to be astringent.

The decomposition substances formed from trigonelline during pyrolysis such as pyridine contribute to the coffee aroma. Up to 75% of the original 0.8% to 1.2% concentration is decomposed depending on the roasting degree. Moreover, nicotinic acid is created. Nicotinic acid belongs to the vitamin B complex.

# 7 CHEMICAL REACTIONS

Fig. 26:  
Development of  
chlorogenic acid  
during roasting

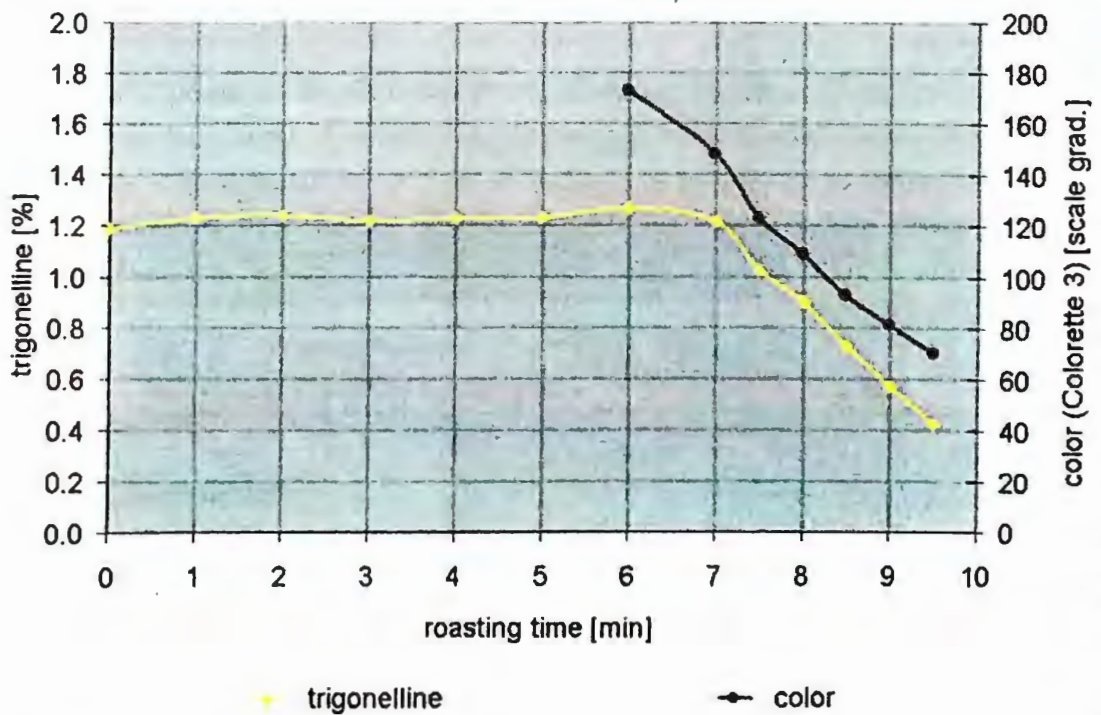
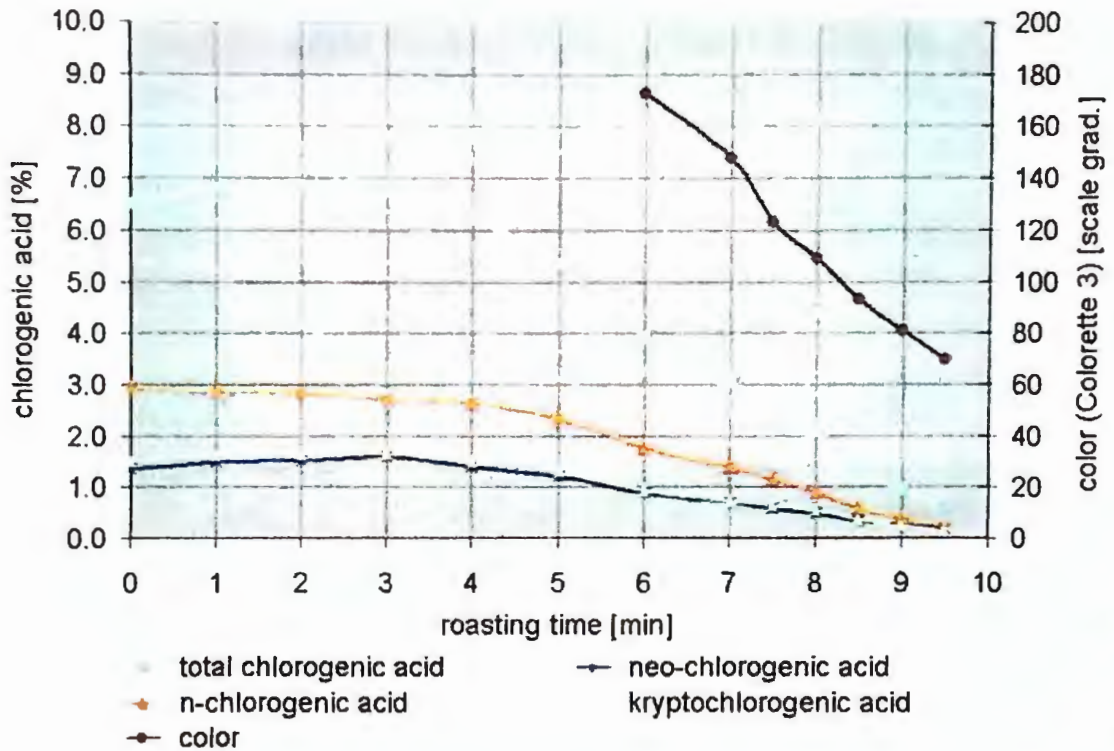


Fig. 27: Development of trigonelline during roasting

Trigonelline decomposition during roasting is shown in Figure 27 using the example of the Columbia sort. Compared to chlorogenic acid decomposition, this decomposition does not happen until later at higher temperatures.

Caffeine is physiologically one of the most effective substances and moreover contributes to the bitter taste profile of the coffee. Caffeine has a relatively stable behavior during roasting. A very minor portion is carried away as vapor, particularly in the final roasting phase. These losses are **overcompensated** by the developing loss of carbon dioxide and carbon monoxide.

The decomposition of the chlorogenic acids (Fig. 28) and trigonelline (Fig. 29) is portrayed in the following bar charts.

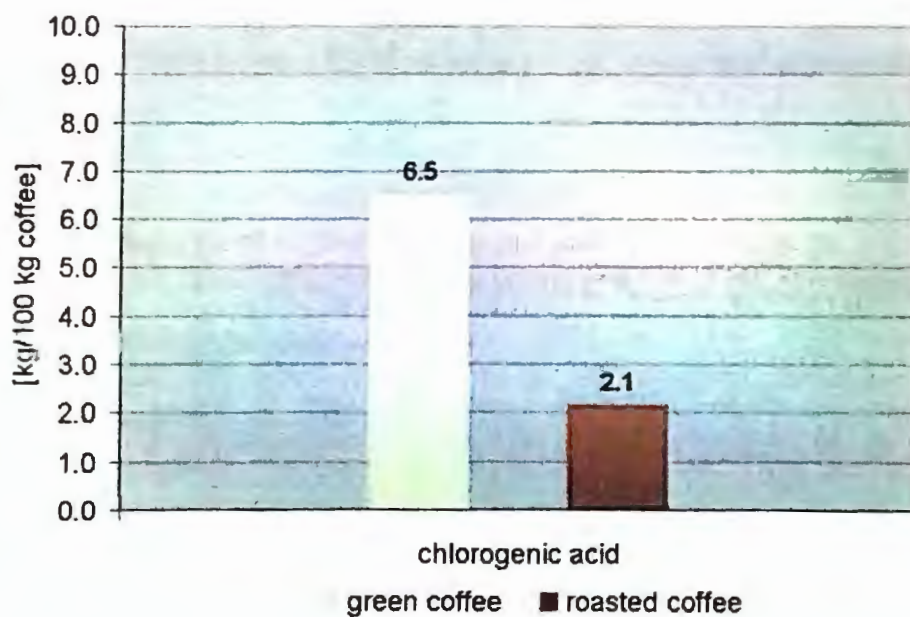


Fig. 28: Chlorogenic acid decomposition

# 7 CHEMICAL REACTIONS

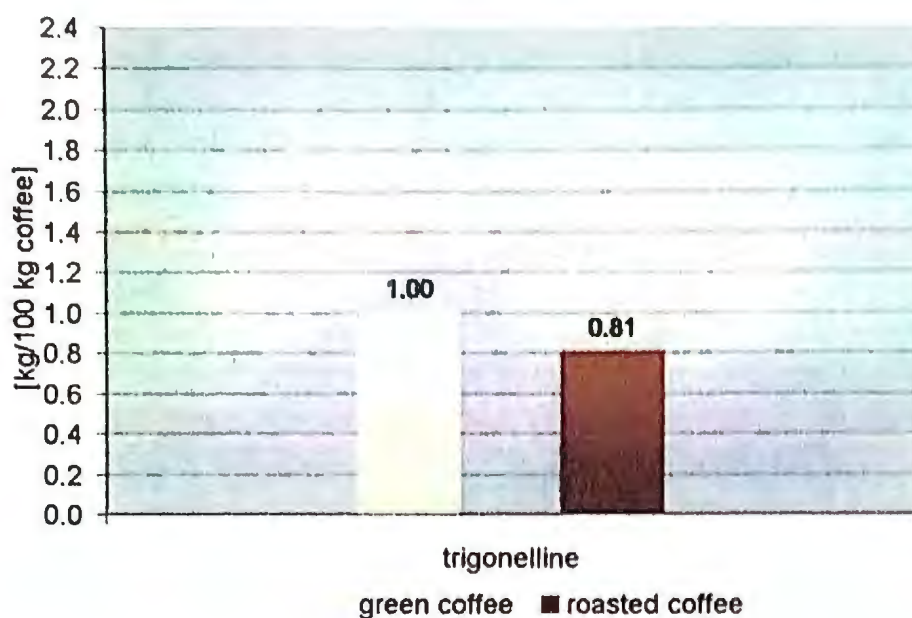


Fig. 29: Trigonelline decomposition

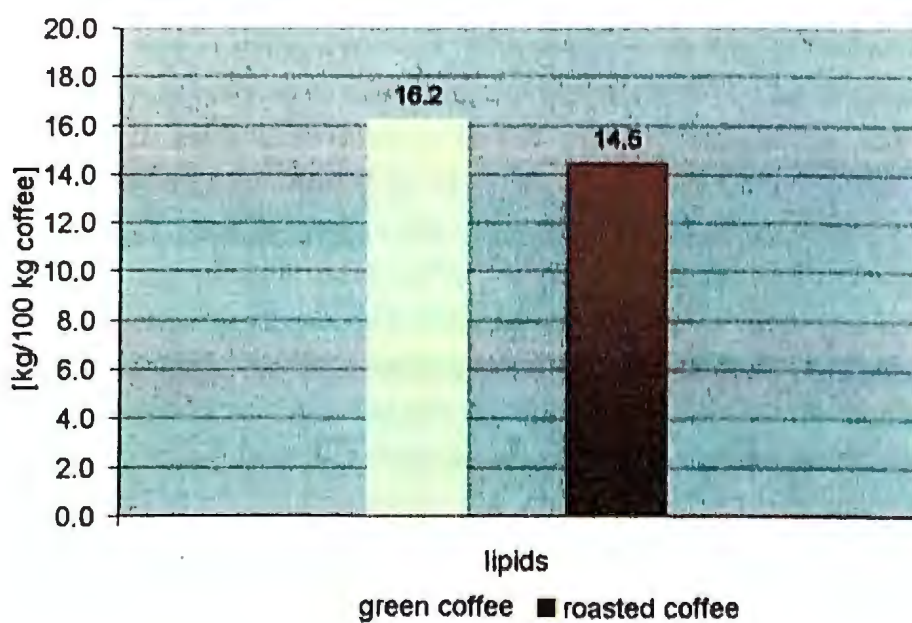



Fig. 30: Lipid decomposition



The non-saponifiable fat fractions of the lipids are broken down into volatile terpenes. The major part of the lipids on hand in green coffee remains unchanged in terms of quantity by the effects of temperature.

The last bar chart (Fig. 30) shows as an example the share of lipids in raw coffee and roasted coffee. Approx. 10% of the lipid share was converted into volatile terpenes und aldehydes.

The contribution pyrolysis makes to aroma development includes – in abbreviated form – the formation of volatile phenols from chlorogenic acid, the formation of pyridines and pyrrolines from trigonelline and the formation of volatile terpenes from the lipids.

The development of the aromatic compounds is for the most part dependent on the roasting degree of the coffee. The roasting degree influences not only the formation but also the decomposition of diverse aromatic compounds.

Some volatile compounds increase in quantity with an increased roasting degree, others in turn increase to a certain roasting degree and subsequently begin to decompose when the roasting degree continues to rise. Over and above this, there are volatile aromatic compounds that after a tendency to increase and decompose, are recomposed in the continued course of roasting.

A typical example of the reaction behavior is shown by the course of the furfural concentration during a roasting process. The maximum furfural concentration is already reached at a very light roasting degree. The continuance of roasting, after a value held more or less constant, brings about a gradual decomposition of this substance (Fig. 31).

Furfural ( $C_5H_4O_2$ ) is regarded as a leading substance for the steam-volatile aromatic compounds of the roasted coffee. Furfural is a heterocyclic compound of furans. Furan produces a pleasant taste which is caramel-like to woody.

The decomposition of certain aromatic compounds is in part attributable to the fact that a portion of these volatile compounds escapes from the coffee beans with carbon dioxide and carbon monoxide by way of the permeable cell wall structure. These released gases are absorbed by the roasting air and discharged as gaseous organic emissions.

## 7 CHEMICAL REACTIONS

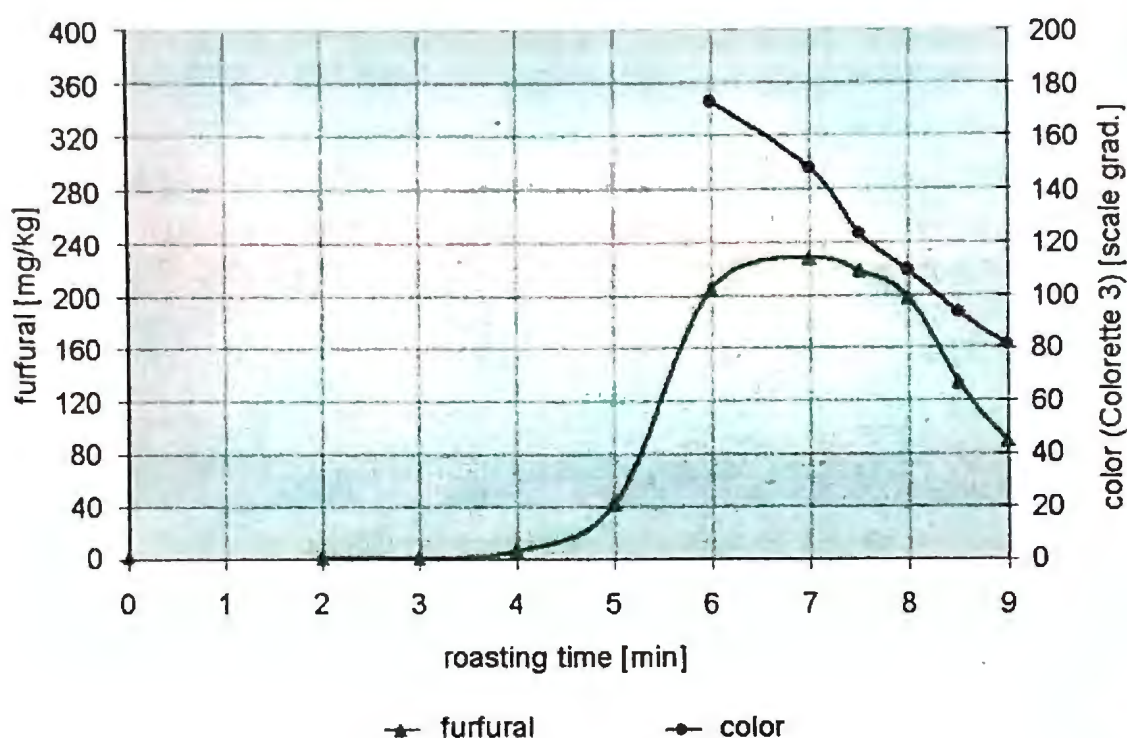


Fig. 31: Development of furfural during roasting

With increasing coffee temperature, the quantity of gaseous compounds being released rises. The concentration of these compounds increases disproportionately as of a specific roasting degree. The increase plotted against the roasting time can be seen in the following graph (Fig. 32). Plotted are the course of the coffee temperature and the course of the carbon concentration ( $C_x$ ). The  $C_x$  concentration represents the concentration of gaseous organic compounds in the roasting process waste gas and corresponds to the total carbon share of the aromatic compounds.

A series of gaseous organic compounds was determined in the roasting process waste gas such as chlorides, furans, nitrogenous compounds, sulfuric compounds, aldehydes, ketones, acids, alcohols and terpenes. Among them, caffeine and acetic acid represented the greatest quantity with a total of approx. 75% to 85%.

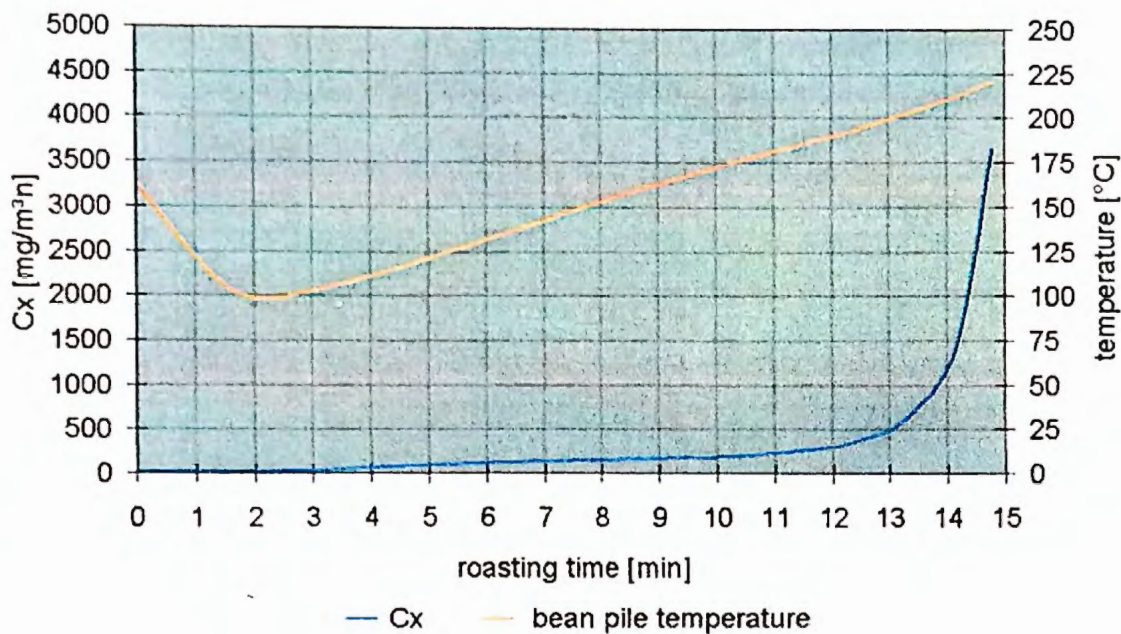


Fig. 32: Roasting process waste gas of batch roaster

Responsible for coffee's acidity are primarily the aliphatic acids such as acetic acid, citric acid, malic acid and phosphoric acid. After the drying phase, the overall acid concentration increases in the lower temperature range and subsequently, in the further course of roasting, again decomposes mainly lightly volatile acids. A great part of the aliphatic acids is already present in the raw coffee. The most important acids in raw coffee are quinic acid, malic acid and citric acid.

Through pyrolysis of the carbohydrates in particular, formic acid, glycolic acid, lactic acid, succinic acid and others are formed. The amounts of quinic acid and phosphoric acid increase during roasting.

## 7 CHEMICAL REACTIONS

The following figure (Fig. 33) shows the initial content of individual aliphatic acids for Columbia coffee and the amounts of acids formed or synthesized through the roasting process.

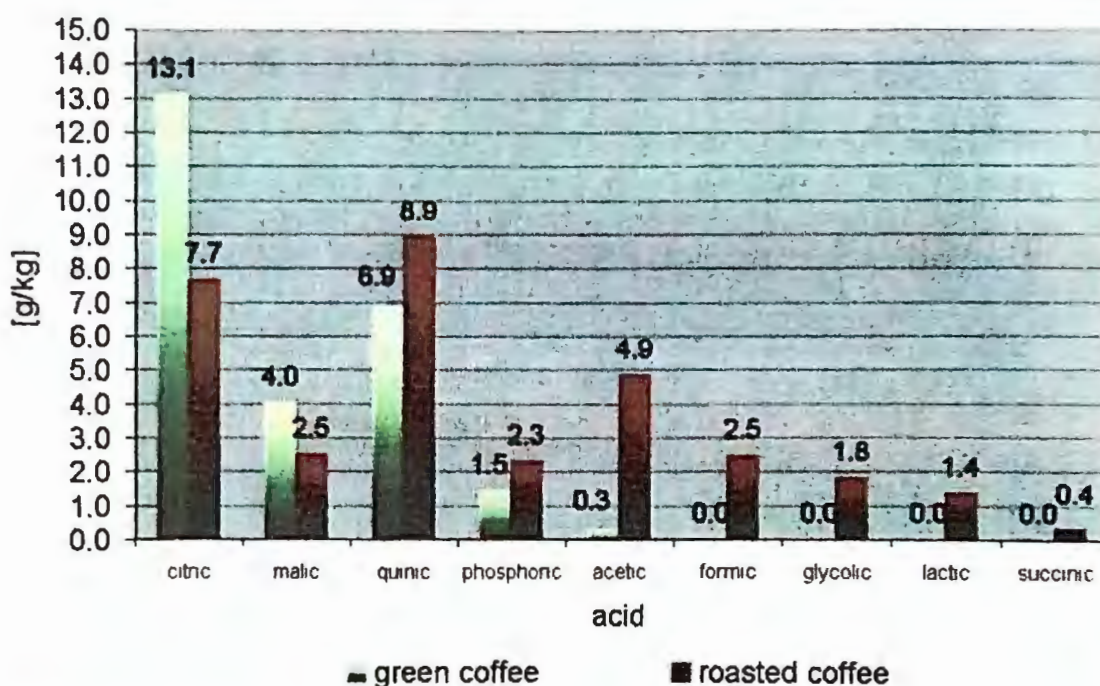


Fig. 33: Aliphatic acids

In the roasted coffee, quinic acid, citric acid and acetic acid constitute the major part of the collective aliphatic acids.

A specific coffee sort, for example, roasted in a specific time at a specific roasting degree contains some 30 g of aliphatic acids per kg of roasted coffee, of which the share of quinic acid is approx. 26%, citric acid approx. 22% and acetic acid approx. 17%. The remaining 35% is dispersed among the many diverse acids.

The gradient of the acetic acid content during the roasting procedure is shown in the following figure (Fig. 34). Approximately midway through roasting, the acetic acid concentration gradually rises to around 1%. The maximum value was reached at a roasting degree of 110 scale degrees. A further reduction of the roasting degree does not lead to a further increase in acetic acid.

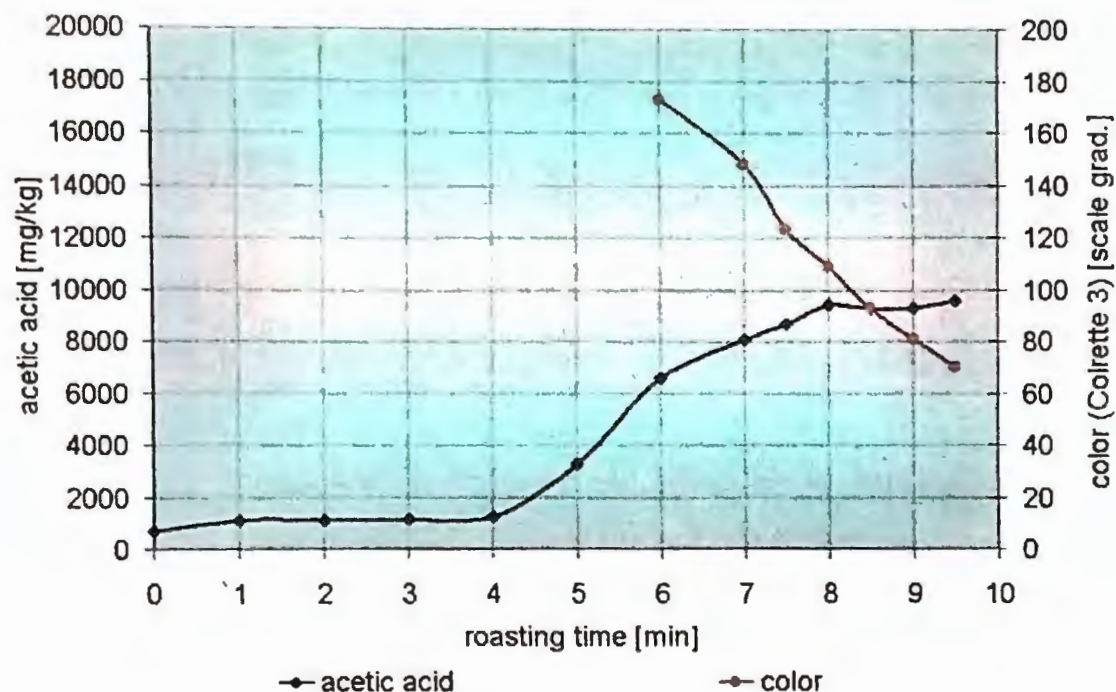


Fig. 34: Development of acetic acid during roasting

The titratable acid index (acid value) is generally accepted in coffee analysis as an assessment of the acidity. A linear relationship arises between the perceived acidity and the acid value. A higher consumption of titrating solution stands for a greater intensity of acidity. To be taken into account, however, is that this is an analytical method that is worked out empirically. The mixture of many different acids, all with their own characteristics, makes it more difficult to make a definitive statement.

The following figure (Fig. 35) illustrates the influence of the roasting process on the formation of acid. This occurs practically simultaneously with the formation of furfural. As of a coffee temperature of approx. 170°C, the acid value begins to sink constantly.

# 7 CHEMICAL REACTIONS

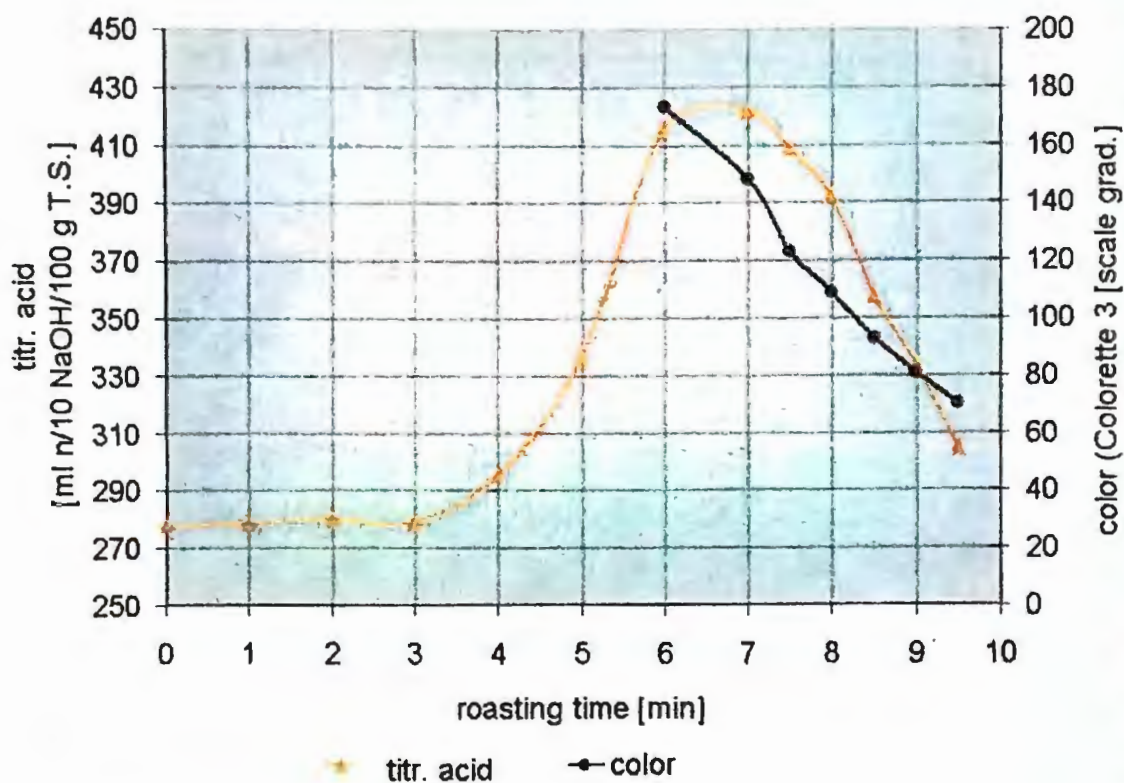
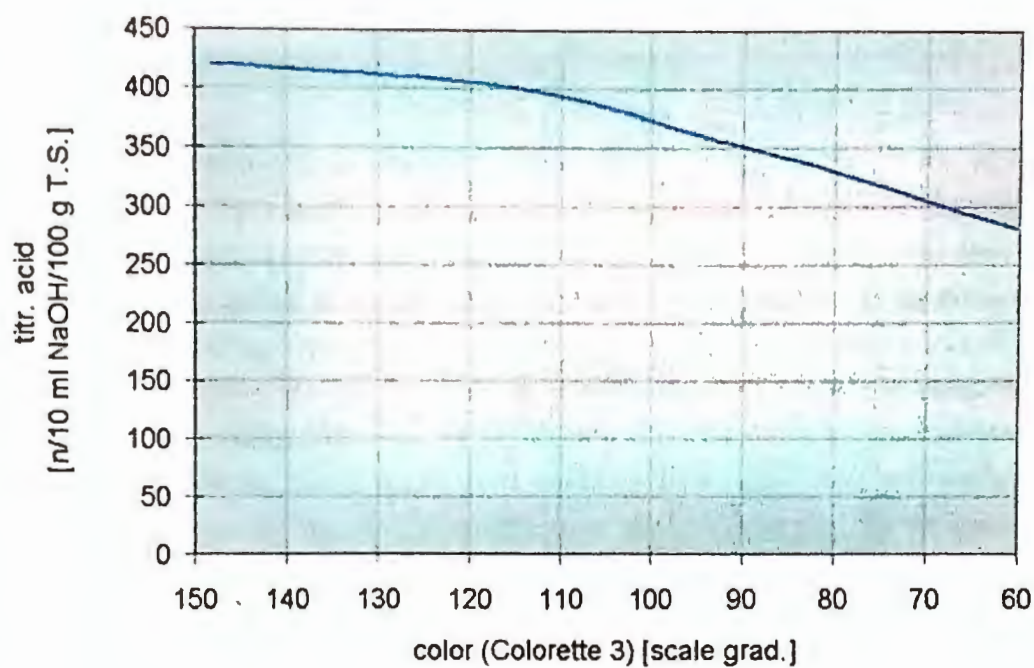


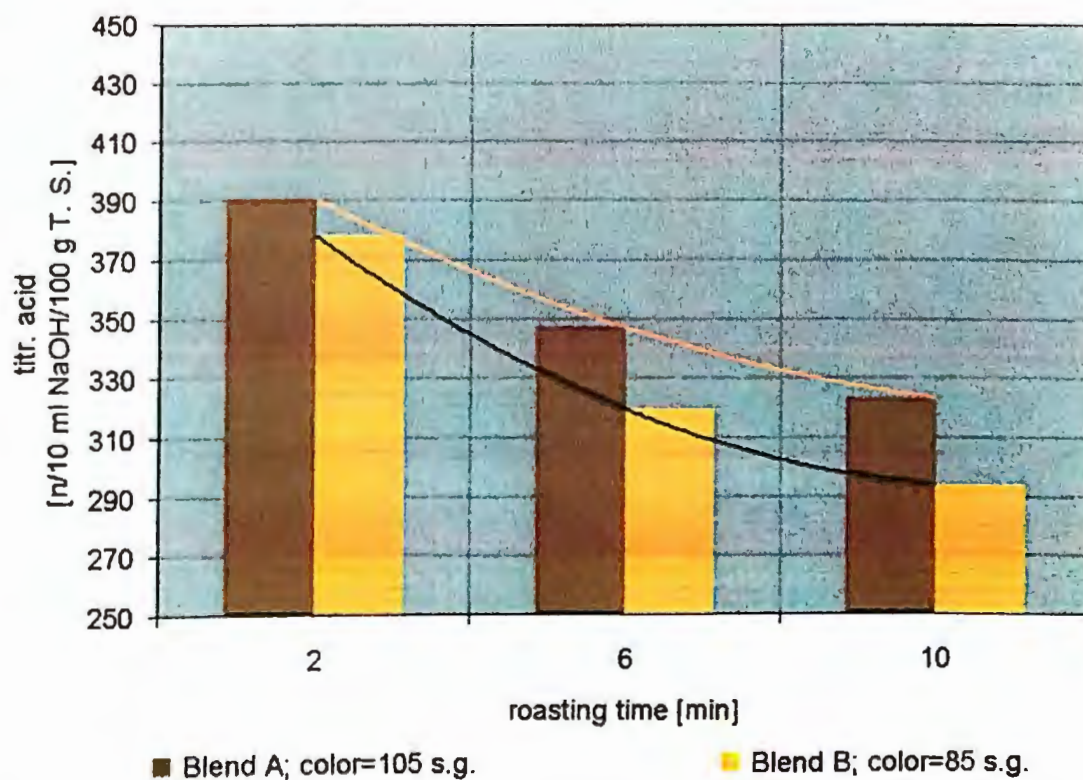
Fig. 35: Development of titratable acid during roasting

As already mentioned, the acid breaks down as the roasting degree increases (lower scale value). The relation between degree of acid on the one hand and color value, i.e. roasting degree on the other hand is shown in the following figure (Fig. 36).

The roasting time also has an effect on the acid content. The tendency that emerges is that the acid content and thereby the acidic taste of the coffee increases with the reduction of the roasting time. The acidity for different roasting times is shown in the following figure (Fig. 37) for 2 different coffee mixtures. Incidentally, the influence of the roasting time on the acidity of light roasted coffees is greater than on dark roasted coffees.



**Fig. 36:** Titratable acids - roasting degree



**Fig. 37:** Titratable acids - roasting time

# 7 CHEMICAL REACTIONS

## 7.4 HYDROLYSIS

Hydrolysis is a chemical reaction in which a chemical compound is decomposed through the action of water. A part of the chlorogenic acids, for example, is converted through hydrolysis into quinic acid and caffeic acid.

The quinic acid present in the raw coffee increases during the roasting process. Unlike acetic acid, the increase takes place already at an earlier stage of the roasting process. After about two-thirds of the roasting time, the color of the coffee, with 180 scale degrees, is very light, and the quinic acid content remains somewhat constant up to a color of 120 scale degrees. Further along in the process, i.e. as the coffee increases in darkness, the quinic acid concentration rises again. At a color of 70 scale degrees, the quinic acid content lies at approx. 3 percent by weight (Fig. 38).

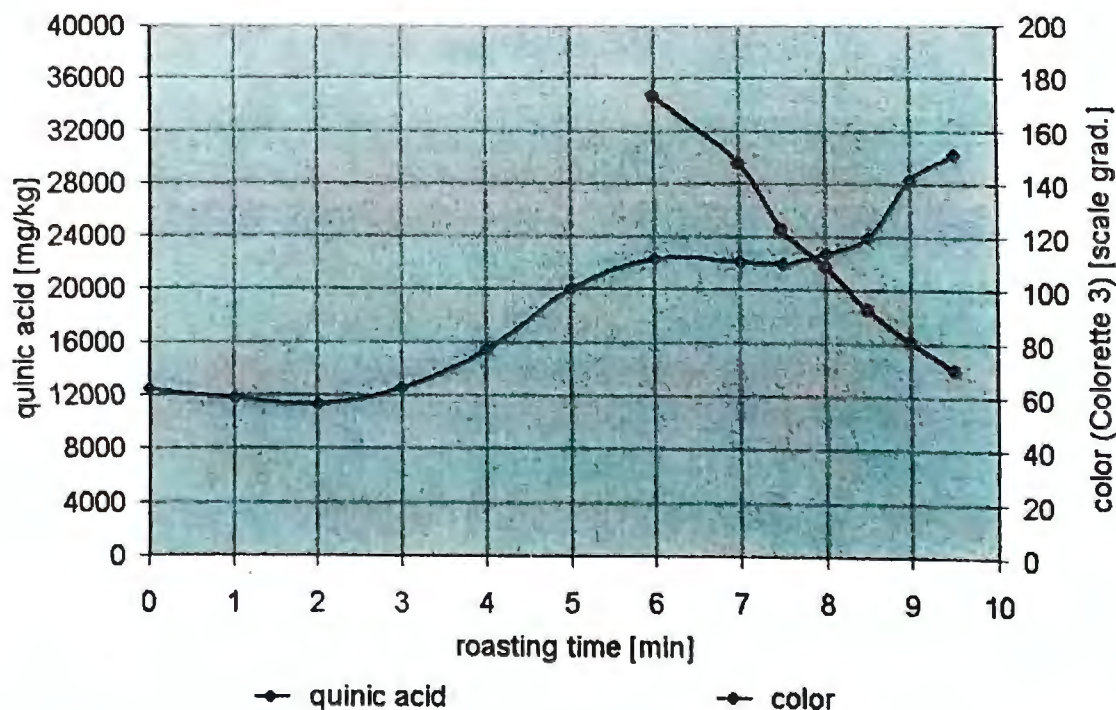


Fig. 38: Quinic acid gradient during roasting

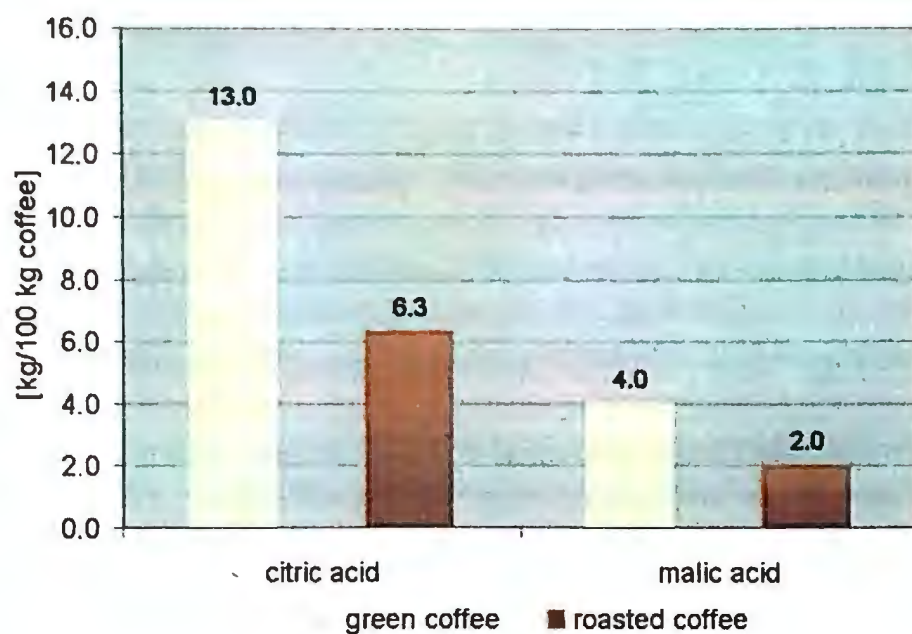


Fig. 39: Decomposition of citric acid and malic acid

In addition, the citric acids and malic acids present in the raw coffee are in part decomposed (Fig. 39). This results in the formation of new acids such as succinic acid, fumaric acid, itaconic acid, citraconic acid and maleic acid.

# 7 CHEMICAL REACTIONS

## 7.5 CONVERSION INTO CARAMEL

Through heating, some of the simple sugars present are caramelized into browning products. These browning products resulting from the splitting off of water belong for the most part to the furan group. A typical example of conversion into caramel is the formation of maltol from fructose. Maltol, i.e. larixinic acid, is a typical, pleasantly caramel-smelling compound which, incidentally, is easily soluble in water, something that cannot be said for all of the caramel products formed.

The caramel products contribute, along with the melanoidins formed in the Maillard reaction, to the brown color of the coffee beans, i.e. the coffee beverage.

## 7.6 OXIDATION

Oxidation is the chemical union of elements or compounds with oxygen. Energy is released in this reaction. In the course of roasting, an oxidation takes place with the non-volatile essential oils. The non-volatile essential oils oxidize in the higher coffee temperature range to volatile aldehydes such as pentanols and hexanol, for example. The amount of aldehydes formed from the oils is very minimal. The aldehydes nevertheless have considerable influence on the actual coffee aroma.

The slight decomposition of lipids during the roasting process occurs not only through oxidation but also through pyrolysis.



## 7.7 DECARBOXYLATION

The development of carbon dioxide and carbon monoxide takes place for the most part through decarboxylation and less through combustion. At coffee temperatures from approx. 195°C, the release of carbon dioxide increases abruptly and water is formed. Through the Maillard reaction, Strecker synthesis, pyrolytic decomposition and oxidation, not only the volatile organic compounds are formed, but also, as a side product, carbon dioxide and carbon monoxide.

In terms of quantity, the mixture comprising nitrogen, carbon dioxide and carbon monoxide far exceeds all of the other volatile substances in the coffee. Due to the formation of steam and gas, the pressure in the cells increases. As a result, the volume of the cells swells and the cellular tissue loosens. Due to the high internal pressure, the major part of the gas that has formed escapes by way of the semi-permeable cell wall and the cracks formed through drying.

A certain percentage of the gas, under a considerable overall pressure, remains in the cells of the coffee beans. This remaining portion of gas can amount to 2 weight percent. Knowledge of the cavity volume and the residual gas quantity for a very specific coffee sort, roasted for a very specific time period at a very specific roasting degree makes it possible to calculate the internal pressure in the relevant cells.

The quantity of gas remaining in the cells immediately subsequent to roasting is also dependent, apart from the coffee sort, on the roasting degree and the roasting time. When the roasting degree is raised and the roasting time reduced, the residual quantity in the coffee bean increases.

An average Arabica coffee, roasted in about 8 minutes at a central European roasting degree of 120 scale degrees (measured with the Colorette 3a color measuring unit) and suitable for filtering, has a gas share of approx. 0.8 percent by weight directly following the roasting and cooling procedure.

As described by Stefan Schenker in his dissertation (ETH No. 13620, Zürich 2000), the released gas mixture after a 4-month storage period for a specific coffee roasted in a roasting time of around 10 minutes comprises 72.8% carbon dioxide, 17.1% carbon monoxide including residual elements, 9% nitrogen and 1.1% argon and oxygen.

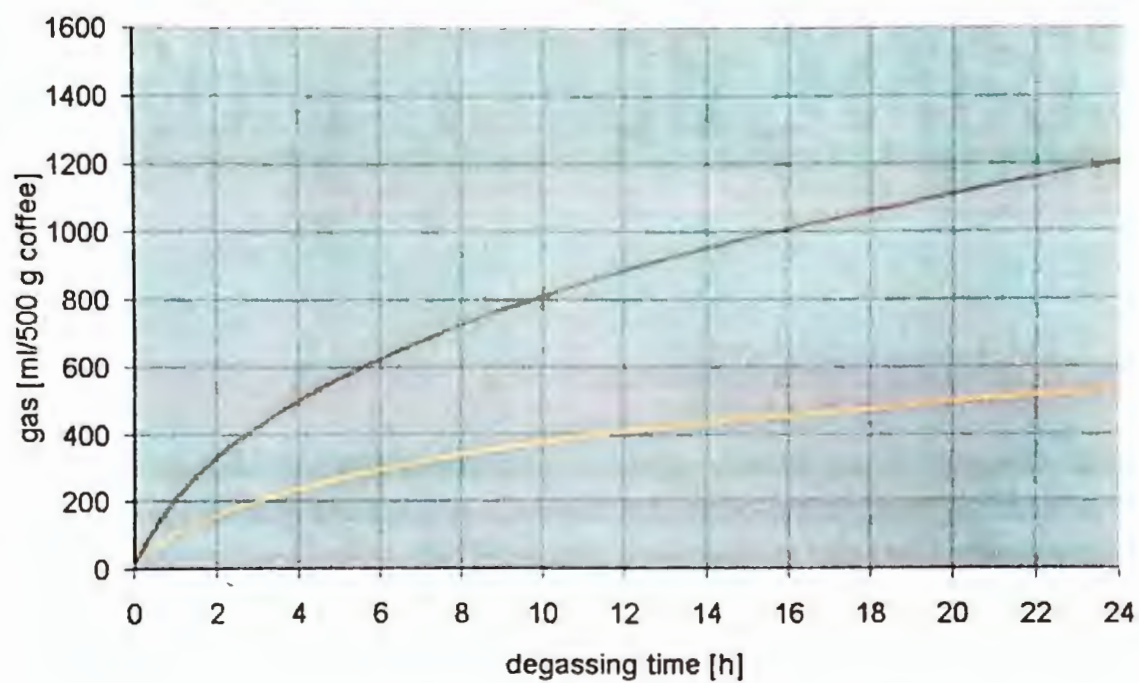
## 7 CHEMICAL REACTIONS

A cell cavity volume proportion (porosity) of 42% and a gas quantity enclosed in the cells of 0.8 weight percent yields an overpressure of approx. 8 bar by calculation. This state refers to whole coffee beans immediately after the cooling process has ended.

In the course of time, the gas enclosed in the cells is released by diffusion until pressure equalization with the surroundings is reached. The speed of degassing for roasted coffee beans is very slow due to the relatively small outer surface and long paths of diffusion. The degassing behavior during the first 24 hours can be seen in the next figure (Fig. 40) for two different roasting degrees.

A total degassing time of 2400 hours until absolute pressure equalization is not unusual. Coffee sorts, roasting degree, roasting time, i.e. the coffee temperature profile during roasting, all have a substantial influence on the quantity of gas produced, on the structure of the cell periphery, on the volume in the cells and thus on the degassing behavior.

Owing to the insignificant quantity of gas remaining in ground coffee, the shorter paths of diffusion and the greater specific surface, the degassing time is shorter by far than for whole coffee beans. Depending on the grinding fineness, a part of the enclosed gas is released immediately in the grinding process through cell destruction. The finer the coffee is ground, the more cells are destroyed and the less gas remains in the coffee particles. Degassing in ground coffee takes place up to a state of equilibrium with the atmospheric ambient pressure, i.e. faster than in whole roasted coffee beans.



color (Col.3) 94 s.g.

color (Col.3) 82 s.g.

Fig. 40: Degassing of roasted coffee beans



## 8 COFFEE BEVERAGE

The method of preparation, i.e. the type of process employed to produce the coffee beverage, has an essential influence on the quality of the beverage. The preparation and the appropriate degree of grinding, i.e. combination of grounds, are responsible for the extraction behavior.

Not every compound present in the roasted coffee bean will be conveyed to the beverage automatically. The most diverse types of preparation, such as the Turkish method, the Greek method as well as methods of preparation for espresso, filtered coffee and the like, all exhibit their particular extraction behavior. Moreover, the quality of the beverage is affected by the dosage, the storage conditions of the coffee, the water temperature and likewise the water hardness. The production of instant coffee occupies a special place in methods of preparation.

In this handbook, the special features of the methods of preparation and their effects will not be gone into any further.



# 9 REFLECTION

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This handbook deals with the physical changes and chemical reactions that take place in the coffee product during the roasting process. Coffee is an important product in global trade and enjoys a great degree of attention not only from business people but also from scientists. A great deal of knowledge about the “inner life” of coffee beans has been gathered up to now and published in a considerable range of books. Since coffee is a popular stimulant, attempts are made again and again to “optimize” the product, or more precisely, to adapt it to constantly changing demands. Hence, the motivation to be thoroughly familiar with the product is high.

Everyone working with coffee endeavors to achieve a product which is attractive to the eyes as well as to the senses. The level of know-how achieved by today's experts is undoubtedly high. Nevertheless, the chemical and physical processes that accompany roasting have not been investigated in their complexity down to the last detail.

Hence every attempt to create an artificial coffee aroma from all of the identified aromatic compounds has been unsuccessful to this day. There are evidently still unidentified aromatic substances in the coffee bean which, although present in hardly measurable concentrations, still have a very effective say in determining the coffee aroma. Or perhaps there are interrelationships between already known constituent substances that have yet to be recognized.

The coffee bean is a complex natural product about whose different components new knowledge is constantly being gained; and this also holds true for the processing of this product. Ultimately, however, uncertainty still looms over the overall connection on how, for example, the changing of a single parameter or substance really effects the coffee plant or coffee bean as a whole.

# 10 APPENDIX



## 10.1 GRAPHICS INDEX

Fig. 1:	Chemical substances in green coffee [% ds]	11
Fig. 2:	Chemical substances in green coffee [% ds]	11
Fig. 3:	Sorption isotherm for raw coffee beans (20°C)	12
Fig. 4:	Temperature development of a coffee bean	17
Fig. 5:	Temperature development of a coffee bean	18
Fig. 6:	Temperature development during roasting	19
Fig. 7:	Heat energy for coffee roasting in kJ/kg green coffee	20
Fig. 8:	Semi-ellipsoid; shape of a coffee bean	23
Fig. 9:	Green coffee bean, Brazil	24
Fig. 10:	Cells, scanning electron microscope	25
Fig. 11:	Cells, scanning electron microscope	26
Fig. 12:	Roasted coffee bean with cracks	27
Fig. 13:	Expansion of coffee beans during roasting	30
Fig. 14:	Expansion of coffee beans	31
Fig. 15:	Roasting sequence	33
Fig. 16:	Loss of substance	35
Fig. 17:	Loss of dry substance during roasting (roasting time approx. 8 min.)	36
Fig. 18:	Development of bulk density during roasting (coffee sort: Columbia)	38
Fig. 19:	Roasting time/bulk density; coffee sort: Columbia	39
Fig. 20:	Development of moisture during roasting	42



Fig. 21:	<b>Residual moisture development depending on roasting degree</b>	44
Fig. 22:	<b>Identified components in roasted coffee</b>	46
Fig. 23:	<b>Carbohydrate decomposition through the Maillard reaction</b>	49
Fig. 24:	<b>Amino acid decomposition through the Maillard reaction</b>	50
Fig. 25:	<b>Protein decomposition through the Maillard reaction</b>	50
Fig. 26:	<b>Development of chlorogenic acid during roasting</b>	52
Fig. 27:	<b>Development of trigonelline during roasting</b>	52
Fig. 28:	<b>Chlorogenic acid decomposition</b>	53
Fig. 29:	<b>Trigonelline decomposition</b>	54
Fig. 30:	<b>Lipid decomposition</b>	54
Fig. 31:	<b>Development of furfural during roasting</b>	56
Fig. 32:	<b>Roasting process waste gas of batch roaster</b>	57
Fig. 33:	<b>Aliphatic acids</b>	58
Fig. 34:	<b>Development of acetic acid during roasting</b>	59
Fig. 35:	<b>Development of titratable acid during roasting</b>	60
Fig. 36:	<b>Titratable acids - roasting degree</b>	61
Fig. 37:	<b>Titratable acids - roasting time</b>	61
Fig. 38:	<b>Quinic acid gradient during roasting</b>	62
Fig. 39:	<b>Decomposition of citric acid and malic acid</b>	63
Fig. 40:	<b>Degassing of roasted coffee beans</b>	67

# 10 APPENDIX

## 10.2 LITERATURE

- 1) Espresso Coffee: The Chemistry of Quality (1995); Hrsg.: Andrea Illy und Rinantonio Viani; Academic Press Ltd., London
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