Roasting Chemistry and Profile Roasting

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Coffee roasting is a chemical reaction process.

Roasted coffee's flavor, aroma and color are created by a <u>multitude</u> of chemical reactions.

Important Roasting Reaction Products and Routes

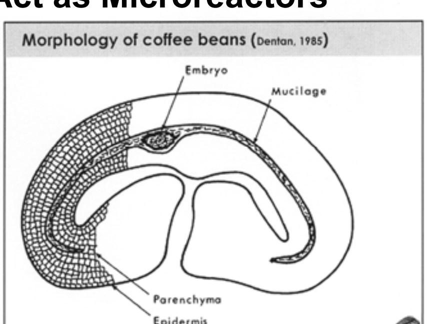
- Pyrazines by α-aminoketone condensations via Maillard reactions (**MR**)
- Diones and furanones via **MR**
- Methional and aldehydes via **MR** and Strecker degradation (SD)
- Sugars and oligosaccharides from cell wall polysaccharide hydrolysis and breakdown
- Aliphatic acids by breakdown of sugars
- Pyridines from trigonelline breakdown

- Damascenone by carotene breakdown, oxidation and isomerizatioh
- 3-methyl indole by oxidative breakdown of tryptophane
- 2-furanaldehyde and 2-furfuryl alcohol via degradation of pentoses
- 2-fururyl mercaptan from the above and H_2S from cysteine or methionine
- Phenolic products, e.g. guaiacol, by breakdown of chlorogenic acids (CA)
- Quinic acid (QA) by CA hydrolysis
- QA and CA lactones by dehydration

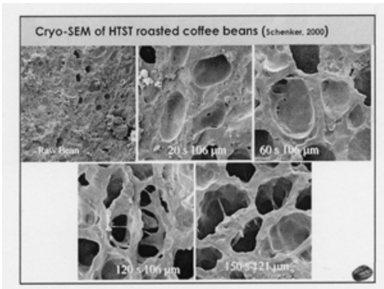
and

hundreds of
other reactions and reaction products

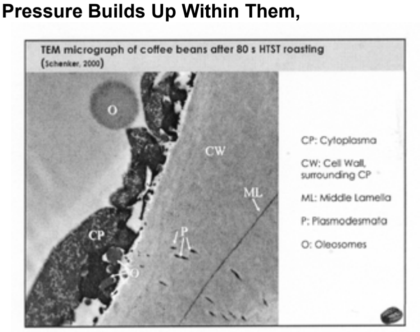
The Cells in Coffee Beans Act as Microreactors



The Cell Walls Act as Walls of Pressure Vessels, Participate In Roasting Reactions, Expand as Internal Water Vapor Pressure Increases, then Stiffen Due to Water Loss



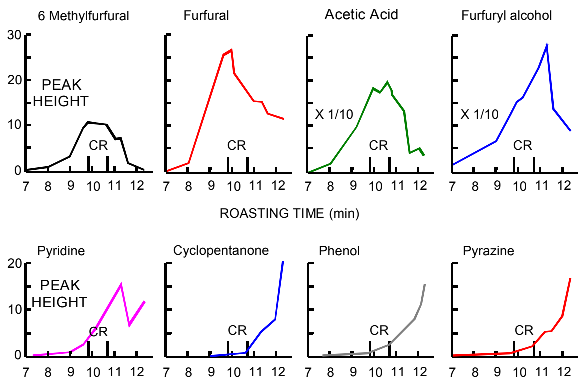
The Cytoplasm and Internal Components of Cells are Driven to Cell Wall Surfaces Early in a Roast. Coffee Oil is Probably Driven into Plasmodesmata, Fine Pores in the Cell Walls, Sealing Them Causing Cells to Retain Gas and Volatile Matter so that Pressure Builds Up Within Them,



Concentrations of roasting reaction products vary strongly with time.

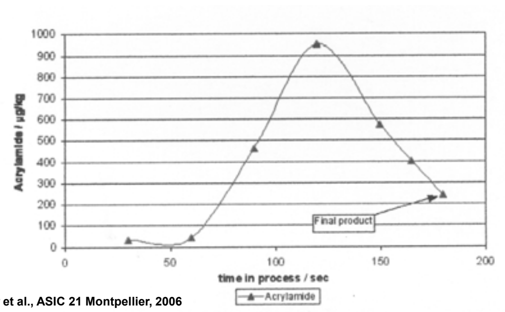
Some peak then decrease.

Others still increase at longer than normal roasting times.

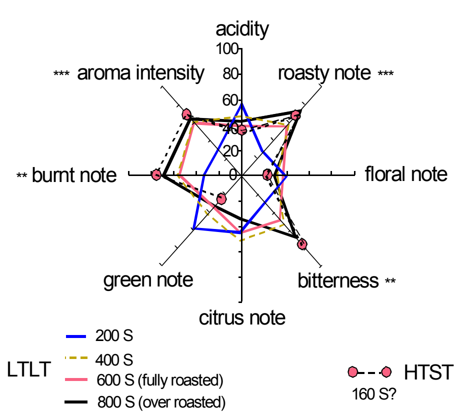


Gianturco

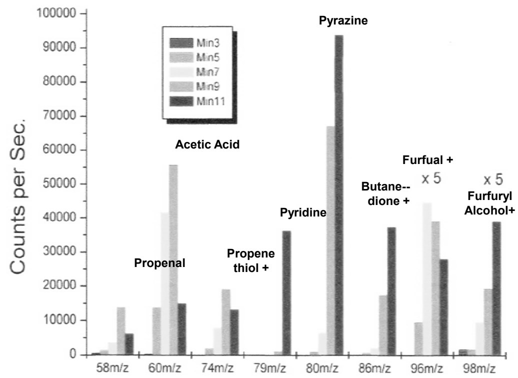
Roasting Reactions also produce undesirable compounds, e.g. acrylamide formed by reactions between reducing sugars and the amino acid asparagine. Like many other roasting reaction products, its concentration peaks during the middle of roasts, then decays as acrylamide is destroyed by other reactions.



Guenther et al., ASIC 21 Montpellier, 2006



S. Schenker Doc. Thesis ETHZ



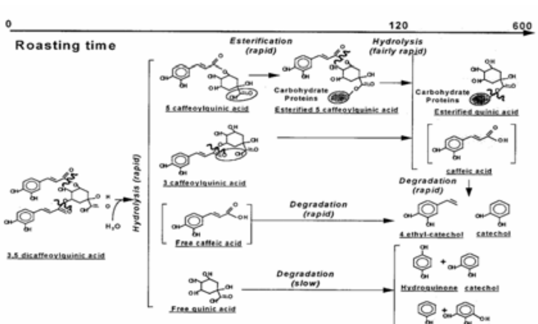
R. Dorfner Thesis University of Munich

Roasting reactions

1.

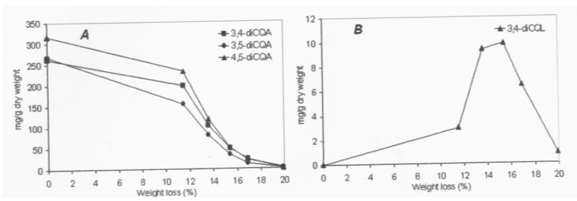
often are complex and involve series of steps and parallel reactions that compete with one another.

Chlorogenic Acids Break Down and The Breakdown Products React with other Coffee Constituents Via A Network of Series and Parallel Reaction Paths

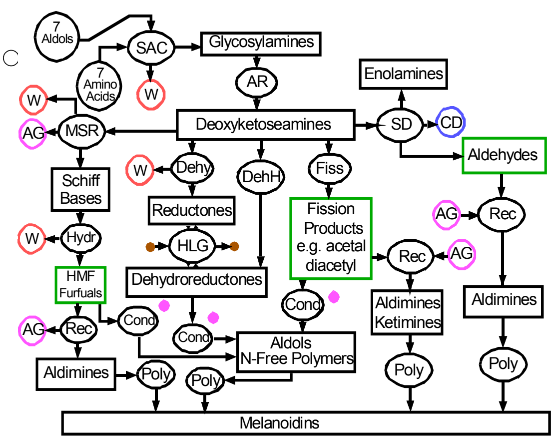


Leloup, Louvrier and Liardon, ASIC 16, Kyoto, 1995

Graph A shows the breakdown of various chlorogenic acids as a function of weight loss during roasting. Graph B shows formation of a chlorogenic acid lactone, a very bitter compound formed by dehydration of chlorogenic acid. The latter reaction is not shown on the preceding reaction scheme diagram. (Note the y scale on graph B is vary much smaller than graph A.)



Moreira, Farah and Donangelo (ASIC 21, Montpellier 2006)



Rates for roasting reactions all tend to increase markedly with temperature, but to markedly different extents.

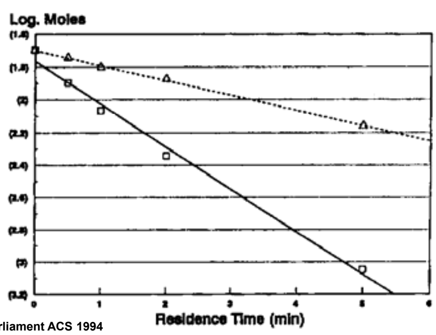
Simple Fist-Order Reaction

A → B $- dC_A = dC_B$

$(C_B)_o = 0$ $C_B = (C_A)_o - C_A$

$$- dC_A/dt = dC_B/dt = kC_A$$

The Logs of the concentrations of Proline (upper curve) and Glucose (lower curve) decrease linearly with time in a constant temperature test modeling the first stage of a Maillard Reaction affecting flavor development during Coffee Roasting. The plot shows characteristic first-order reactant concentration behavior.

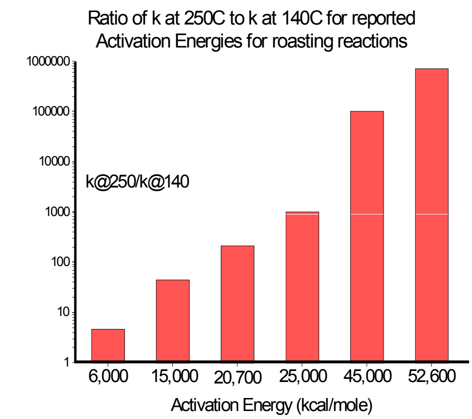


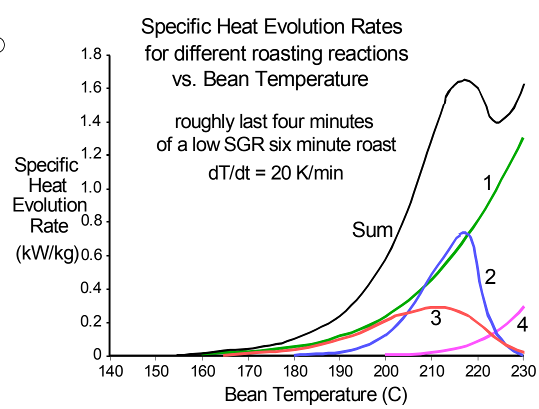
Stahl and Parliament ACS 1994

Effect of Temperature

$$k = A\exp[-E_A/(RT)]$$

A = prefactor
R = gas law constant
$\boldsymbol{E_A}$ = Activation energy
T = absolute temp. (K)

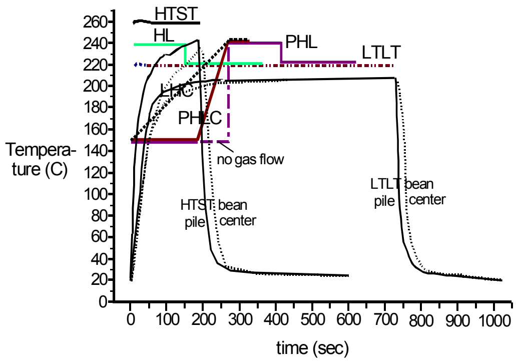




Bean temperature versus time histories during roasting are called <u>bean temperature profiles</u>

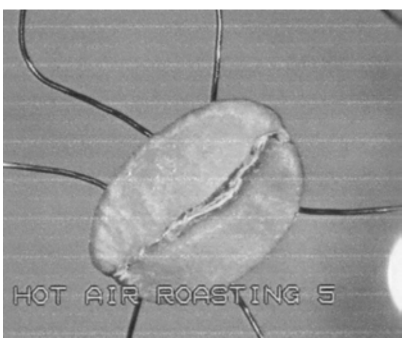
Different temperature profiles cannot provide exactly equivalent roasting results.

Gas Inlet and Bean Temperature Profiles

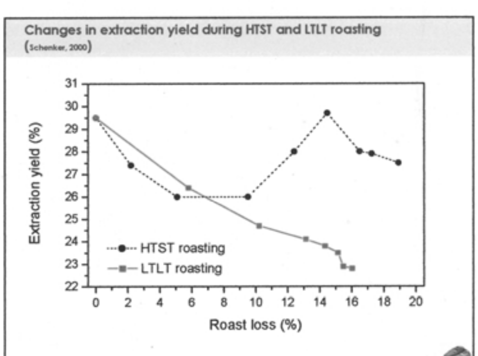


S. Schenker, ETH, Zurich

Bean center temperatures were measured for the HTST and LTLT roasts using this thermocouple arrangement

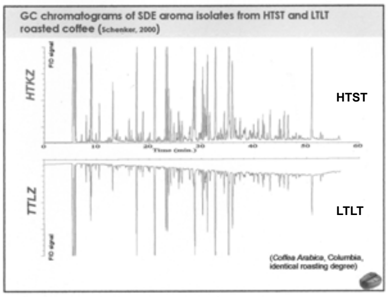


Perren 2008



S. Schenker Ph.D, Thesis ETH Zurich

Comparison of chromatograms for SDE aroma isolates from HTST and LTLT roasts



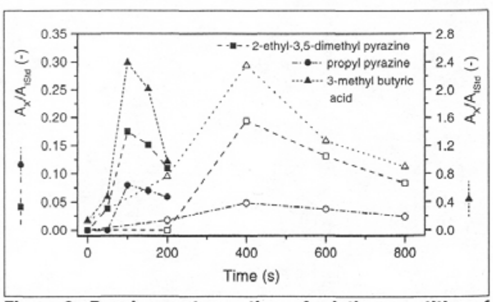
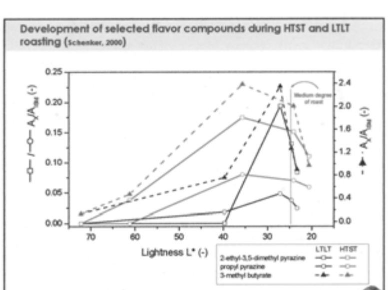
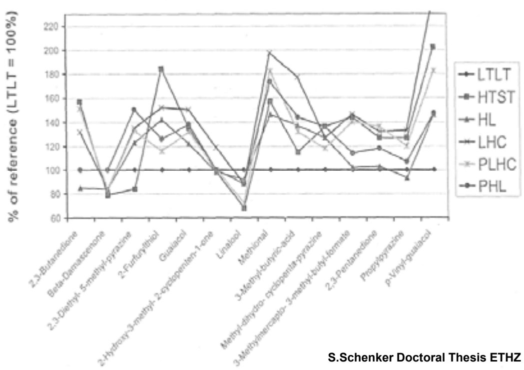


Figure 2—Development over time of relative quantities of 3 selected aroma impact compounds during HTST (solid symbols) and LTLT (open symbols) roasting. Sampling took place at 1/3, 2/3, 3/3, and 4/3 of the normal roasting time to achieve a medium degree of roast.

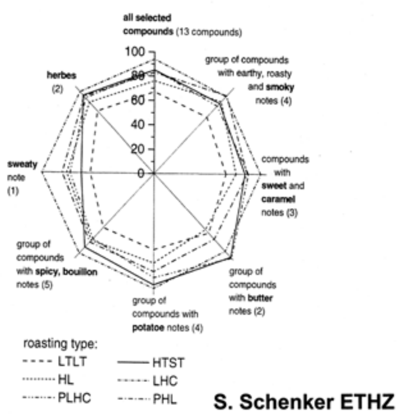
S. Schenker et al. J. Food Science 2002

This shows a composition versus CIE L roast color values. Equal roast colors on the CIE L scale do not provide similar bean chemical compositions.

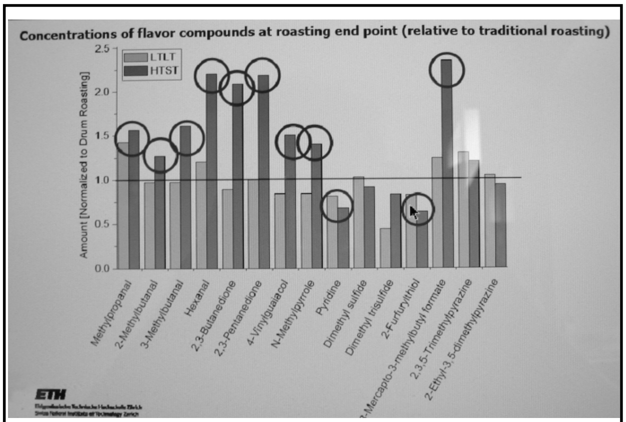




S.Schenker Doctoral Thesis ETHZ

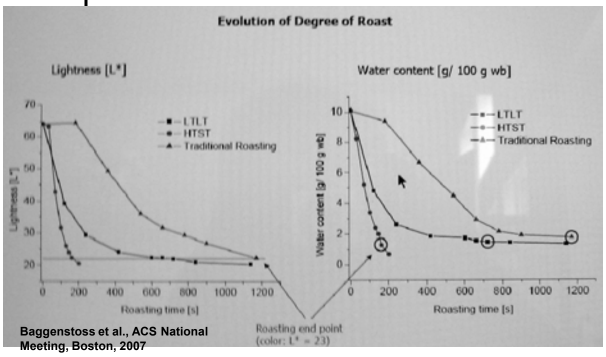


S. Schenker ETHZ



Baggenstoss et al., ACS National Meeting, Boston, 2007

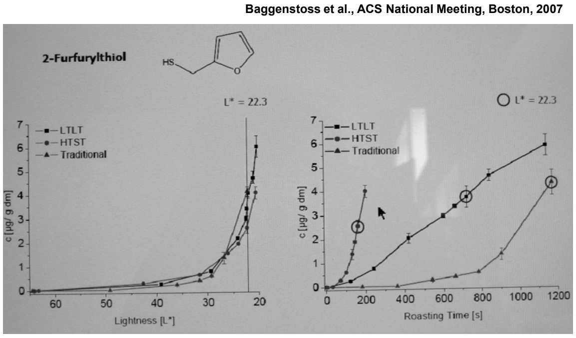
Comparison of roast color and bean water content histories for three types of roasts



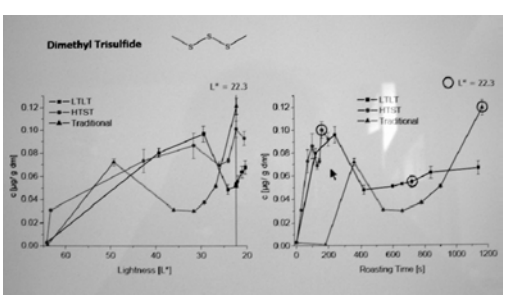
Baggenstoss et al., ACS National Meeting, Boston, 2007

Concentration variation for 2-Furfurylthiol during three type of roasts.

Baggenstoss et al., ACS National Meeting, Boston, 2007

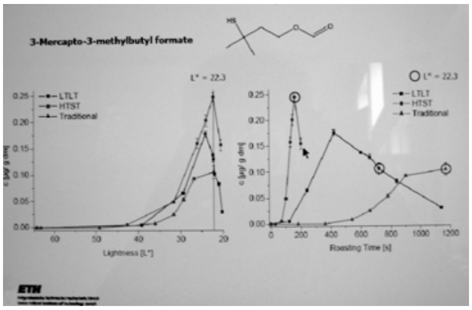


Concentration variation for Dimethyl Trisulfide during three type of roasts.



Baggenstoss et al., ACS National Meeting, Boston, 2007

Concentration variation for 3-Mercapto-3-methylbutyl formate during three type of roasts.



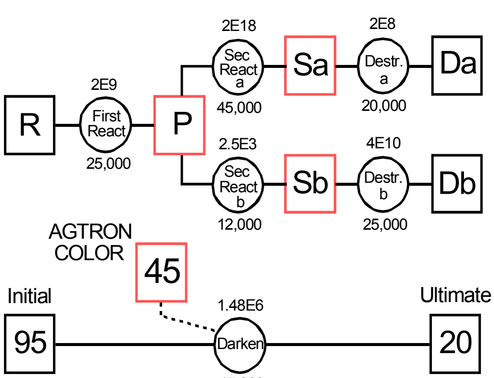
Baggenstoss et al., ACS National Meeting, Boston, 2007

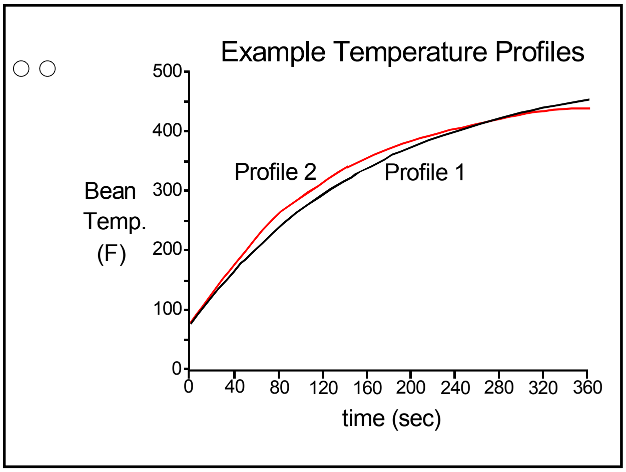
Columbians Roasted to Same Roast Color in Modified Burns Sample Roaster

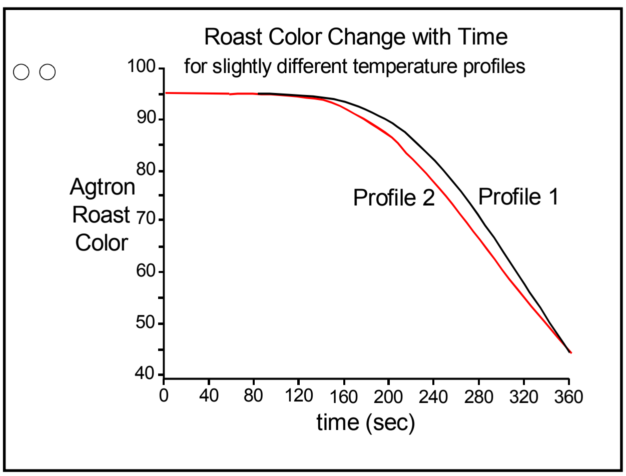
	Time (min)	Temp (F)
A	26	365
B	18	380
C	15	395
D	12.5	410
E	10	425

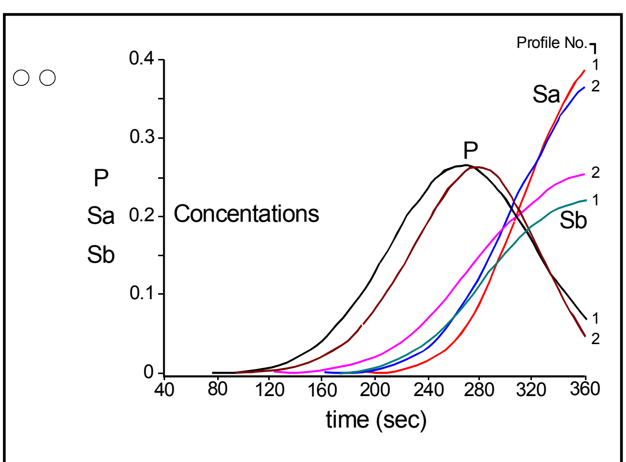
Significantly different pairs
A-D, A-E, B-C, B-D, B-E, DE

Little at. Al.* (1959) Food Technology *U. Calif. Berkeley




Example Temperature Profiles
Bean Temp. (F)
500
400
300
200
100
0
Profile 2
Profile 1
0
40
80
120
160
200
240
280
320
360
time (sec)

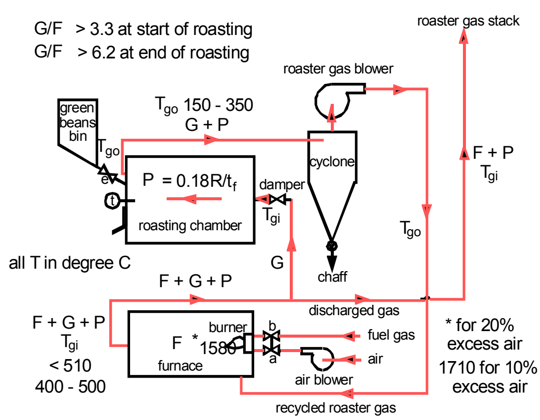

Roast Color Change with Time
for slightly different temperature profiles
Agtron Roast Color
100
90
80
70
60
50
40
Profile 2
Profile 1
0
40
80
120
160
200
240
280
320
360
time (sec)


Profile No.
P
Sa
Sb
Concentations
0.4
0.3
0.2
0.1
0
Sa
P
Sb
1
2
2
1
1
2
40
80
120
160
200
240
280
320
360
time (sec)

In most roasters profiles are roughly controlled by one or two stepwise adjustments* of heat input

* (usually heat input reductions)

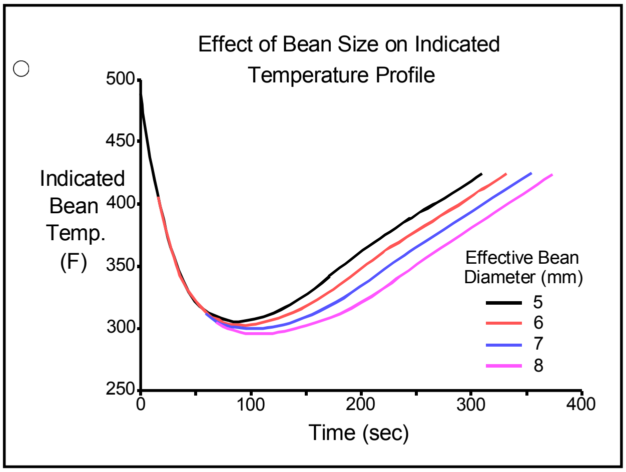
i.e. combustion air and fuel flows to the burner are reduced; and thus F, the burned gas flow rate, decreases

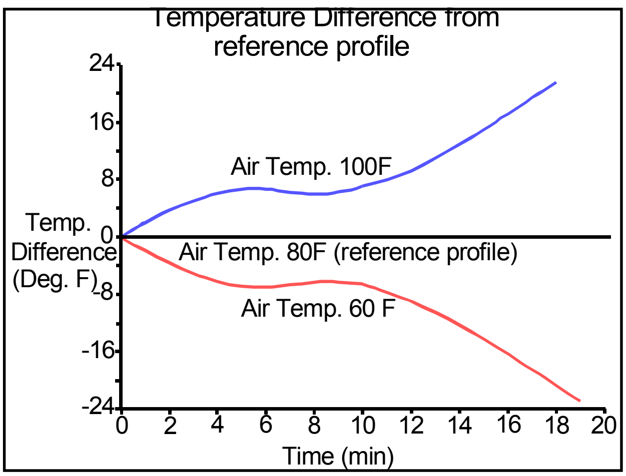


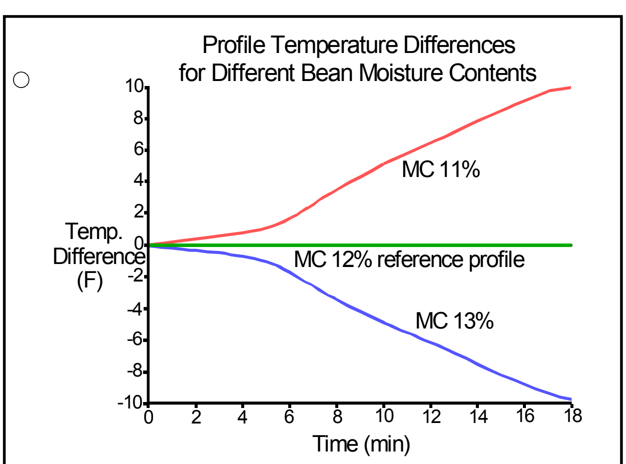
In normally controlled roasters, changes in

- **bean properties,**
- **load size**
- **climatic conditions and**
- **roaster operating conditiona\s**

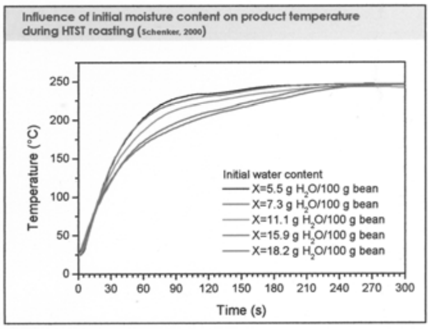
affect bean temperature profiles.

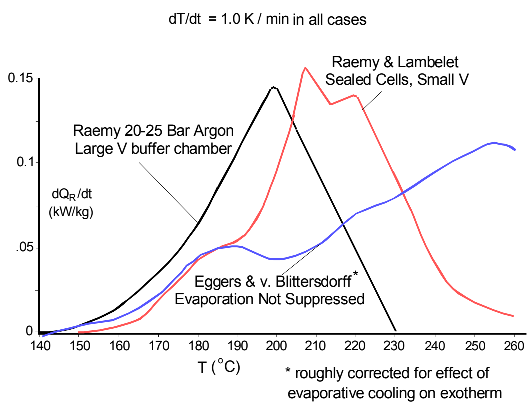

Effect of Bean Size on Indicated Temperature Profile
Indicated Bean Temp. (F)
500
450
400
350
300
250
0
100
200
300
400
Time (sec)
Effective Bean Diameter (mm)
5
6
7
8

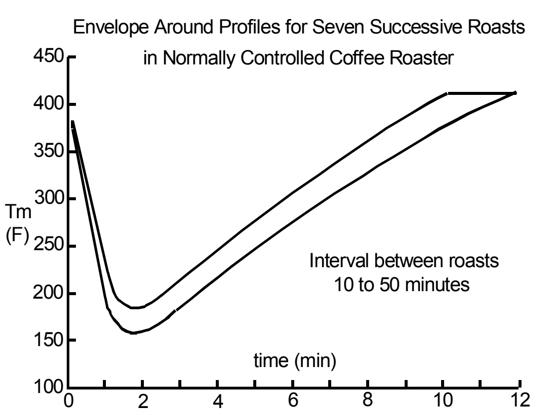

Temperature Difference from reference profile
24
16
8
0
-8
-16
-24
Temp. Difference (Deg. F)
Air Temp. 100F
Air Temp. 80F (reference profile)
Air Temp. 60 F
0
2
4
6
8
10
12
14
16
18
20
Time (min)


Profile Temperature Differences for Different Bean Moisture Contents
10
8
6
4
2
0
-2
-4
-6
-8
-10
Temp. Difference (F)
MC 11%
MC 12% reference profile
MC 13%
0
2
4
6
8
10
12
14
16
18
Time (min)

Effects of initial bean moisture content on bean temperature profile in fluid bed roaster







By controlling the bean temperature profile one can for any given type or blend of coffee beans

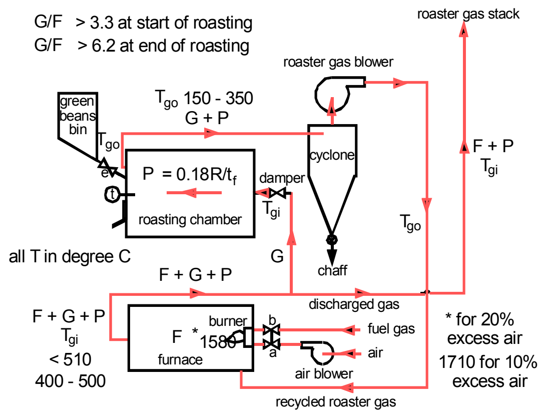
- **a) control attainable roasting reaction outcomes and roasted coffee's character, i.e. flavor, aroma and color; and**
- **b) consistently produce roasted coffee of identical character.**

Roast character, of course is affected by the type of beans used and their composition.

It also depends on bean properties that affect rates of diffusive loss of reactants and reaction products and

may be affected by atmospheric conditions.

Analyzing factors affecting profile control



R = bean load weight

C_B = bean heat capacity

G = gas mass-flow rate

C_G = gas heat capacity

T_B = bean temperature

T_G = gas temperature

F = burner mass flow rate

P = evolved gas & vapor mass flow rate

T_F = burner temperature

T_G subscripts: i = flowing into roaster

o = flowing out of roaster

$$RC_B(dT_B/dt) = GC_G(T_{Gi} - T_{Go})$$

$$- Q_{evap} + Q_{react}$$

$$- Q_{metal} - Q_{lost}$$

Q neglected for control analysis

$$RC_B(dT_B/dt) = GC_G(T_{Gi} - T_{Go})$$

Beans are well mixed in roasters

$$(T_{Gi} - T_{Go}) = E(T_{Gi} - T_B)$$

E = Heat-transfer efficiency

As $E \rightarrow 1$ $\quad T_{Go} \rightarrow T_B$

As $E \rightarrow 0$ $\quad T_{Go} \rightarrow T_{Gi}$

$$(dT_B/dt) \equiv T_B' = [EGC_G/RC_B](T_{Gi} - T_B)$$

Heat-Transfer Efficiency

E = Heat-transfer efficiency

$$E = (T_{Gi} - T_{Go})/(T_{Gi} - T_B)$$

As $E \rightarrow 1$ $\quad T_{Go} \rightarrow T_B$

As $E \rightarrow 0$ $\quad T_{Go} \rightarrow T_{Gi}$

Feedback control is used in modern profile control systems.

The controlled variable is adjusted to minimize (virtually eliminate) differences between the current temperature profile and a reference profile.

In Praxis systems, reference profiles are generated when the system is its learning mode.

Control Options

1) Adjust G
2) Adjust T_{GI}
3) Adjust or control G and T_{GI}

Option 1 $G = V G\rho$

V = blower volume flow rate
ρ = gas density in blower

Adjusting a roaster operating condition affects other operating conditions and profile control response speed.

Example:

Option 1 Adjusting G

Adjusting G causes T_{GI} to change

e.g. in setup shown

$$T_{GI} = (GT_{Go} + FT_F)/(G + F)$$

$$\Delta T_{GI} = - \Delta G(T_{Gi} - T_{Go}) /(G + F)$$

ΔT_{GI} partially cancels effect of ΔG

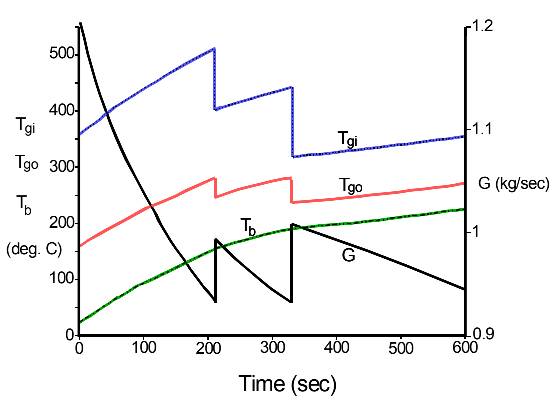
Praxis proportionally adjusts F to keep T_{Gi} constant when G is adjusted.

Such anticipatory control eliminates important control interactions, improving control response accuracy and speed.

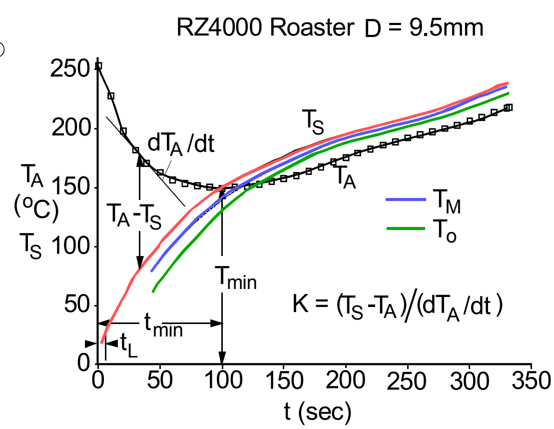
Option 2: Adjusting T_{Gi}

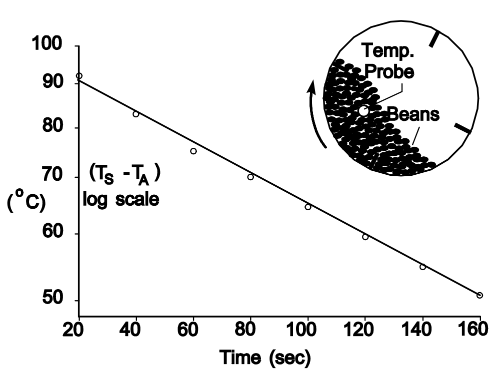
T_{Gi} is adjusted by adjusting F.

Interactions also occur when this is done.



- **Roasting reactions depend on the actual bean temperature path. Profile roasting controls the measured bean temprature path, which is markedly different. But effective control of the actual temperature path is obtained.**
- Corrections can be made for changed differences between measured and actual paths when needed, e.g. as occurs when switching the type of roaster used.



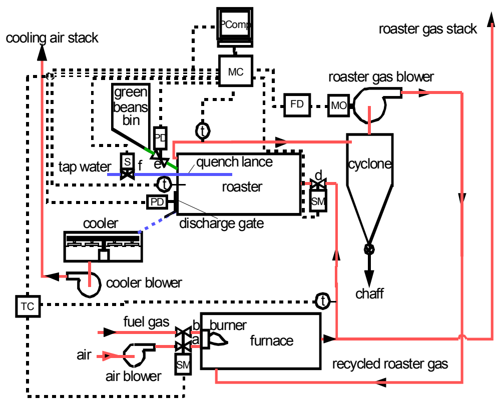


Praxis

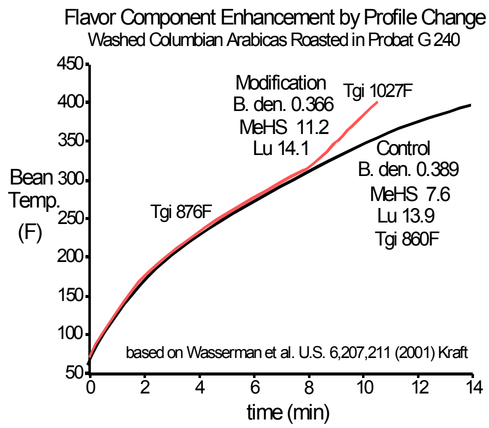
provides conformity between the current measured T_B profile and a learned reference profile by feedback-based adjustment of blower speed, thereby adjusting G

controls T_{Gi} to provide long-range profile adjustment and stability

uses anticipatory adjustment of F to prevent G - T_{Gi} interaction



- **Profile control systems can be used to:**
- **a) provide profiles unobtainable by other control methods;**
- **b) provide particular flavor attributes; and**
- **c) vary roasting speed over wider than normal ranges.**



- Profile roasting systems have data logging and computing capability that can be used to:
- 1) detect when roaster or product behavior tend to change with: a) time; b) climatic condition change; or c) feed properties variation; and
- 2) analyze how these changes and possible causes are related.

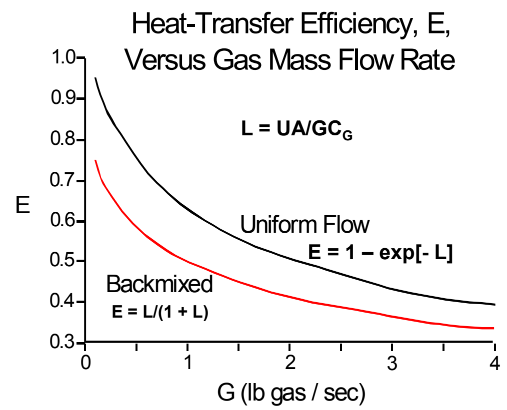
Thus the systems can be used to learn how to adjust roaster operation to compensate for such changes.

Heat-Transfer Efficiency

$$E \equiv (T_{Gi} - T_{Go})/(T_{Gi} - T_B)$$

As $E \rightarrow 1$ $\quad T_{Go} \rightarrow T_B$

As $E \rightarrow 0$ $\quad T_{Go} \rightarrow T_{Gi}$



Summing up:

Controlling bean temperature profiles, lets you:

control roasting reactions

always reproduce your best roasts

with Praxis Logofile systems you can:

1) do this reliably and safely;
2) extend profile and roasting capability,
3) learn how your roaster is working and
4) optimize roasting outcomes.