Engineering A Good Cup of Coffee

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AIChE Mid-Michigan Chapter

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Applied Chemical Engineering

- From Wikipedia:

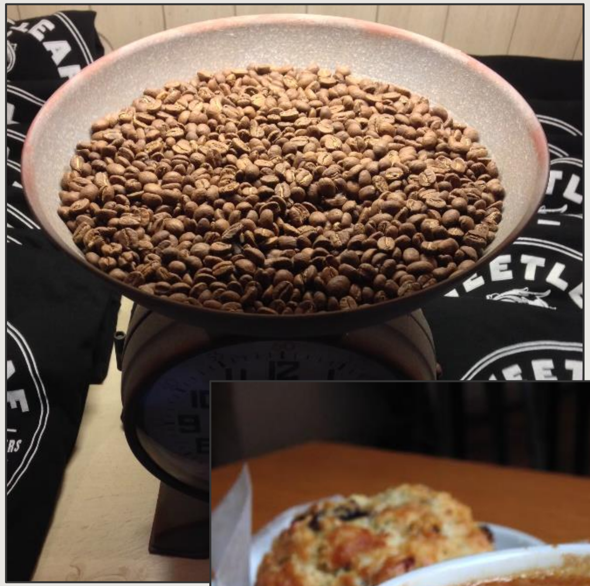
  "Chemical engineering is a branch of engineering that applies to physical sciences and life sciences together with applied mathematics and economics to produce, transport, and properly use chemicals, materials, and energy."

- In other words:

  We can leverage the differences in **physical and chemical properties of different compounds** to yield separations and extractions of energy and mass.

- **What do you think of when you hear the term?**
  - Giant reactors?
  - Distillation columns?
  - Complicated math?

Engineering is Scary, Coffee is Awesome



- Engineering is often seen as a somewhat **opaque** field. But it shows up in nearly **every facet of our everyday lives.**
- While we *could* talk about any number of common chemical products, let's talk about something a little more tasty : **coffee.**
- **Coffee is one of the most prolific beverages on the planet.**
  - 1/3 per-capita consumption of water in US/Europe
  - 10 million tons produced per year globally
  - Responsible for 'survival' of graduate students worldwide

A Brief History of Coffee

- Yes, coffee is a unique and fascinating confluence of many different elements of **cooking and chemistry.**
  - **1st Wave (1800's – mid 1900's)**
    - **Industrialized Commoditization**
    - Bulk-brewed, mass production
  - **2nd Wave (1960's-2000's)**
    - **Branded large-scale chains**
    - Coffee shop culture

A Brief History of Coffee

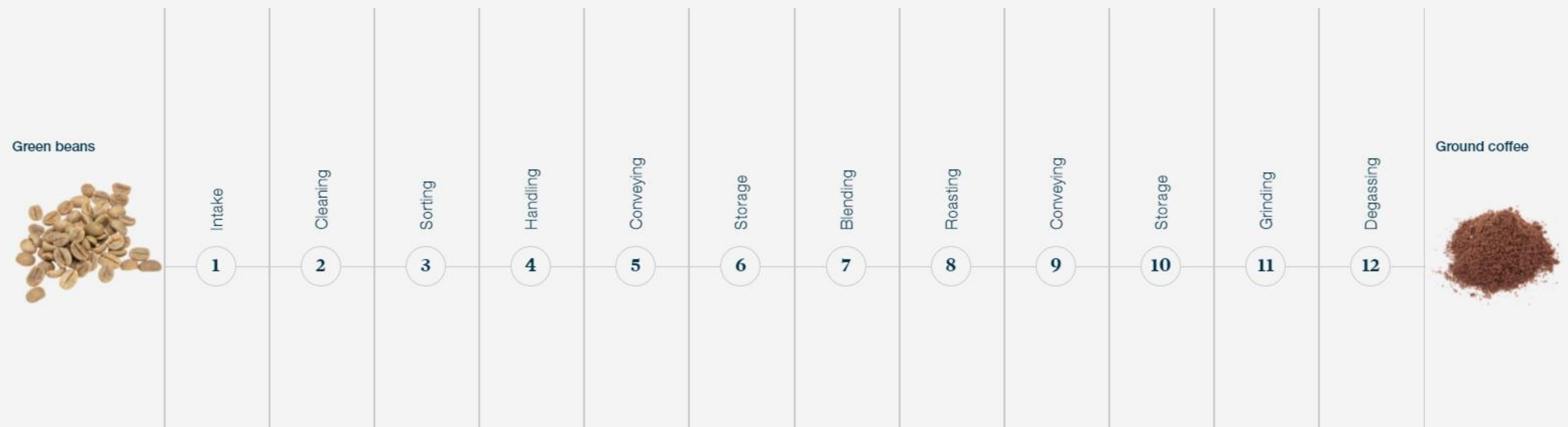
- Yes, coffee is a unique and fascinating confluence of many different elements of **cooking and chemistry.**
  - **3rd Wave (mid 1990's – 2010's)**
    - **Artisanal coffee**
    - Small-batch crafting, sourcing, and production
  - **4th Wave (2010's – now)**
    - **Refocused growth and globalization**
    - Combining the art and science of coffee
  - *Up for debate: a recent **5th Wave**, focusing on craft coffee business practices.*

Coffee in an Industrial Context

Source: Bühler Group.

- **Coffee is the seventh most traded agricultural commodity crop globally, and the second most traded commodity exported by developing countries.**
- The globally high demand of coffee necessitates large-scale processing – not only between ground beans and final beverage as we think of at home, but from **crop to cup.**

Coffee in an Industrial Context



There are a **lot** of steps from beans to finished product!

Source: Bühler Group.

How does coffee utilize chemical engineering concepts?

- The basics of the **engineering design process**
- **Mass and energy balances**
- Competing **reaction and extraction** effects
- Circumventing limitations of **scale-up** and **implementation**

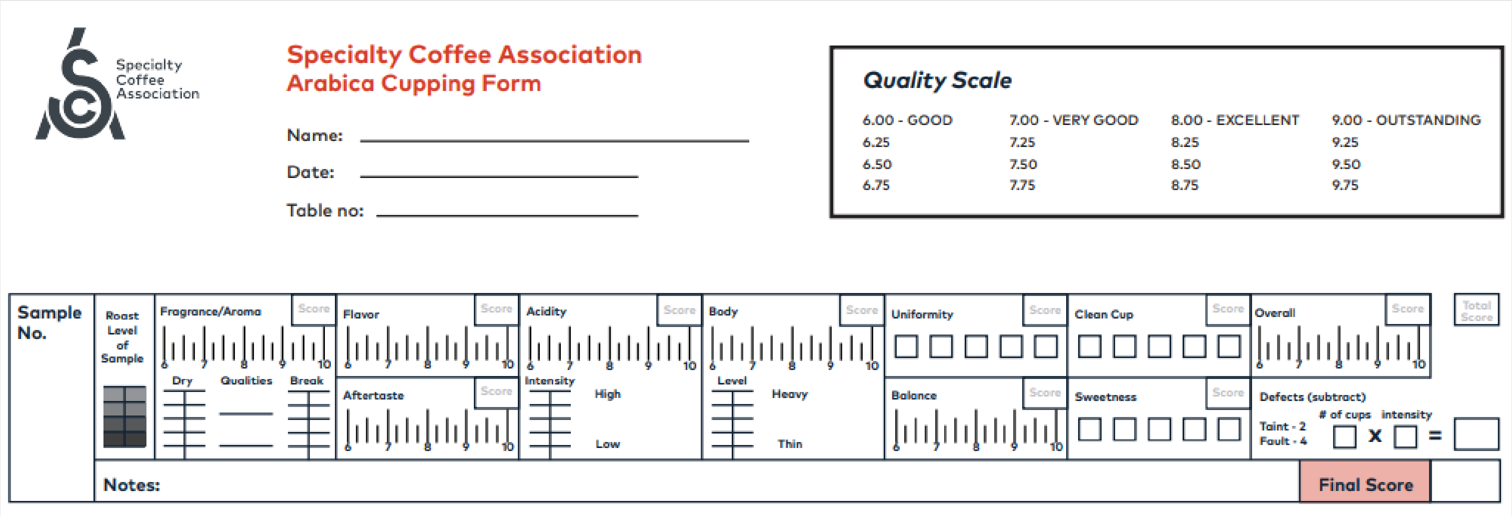
Source: Bühler Group.

Identifying Design Objectives

- Like many food-based products, **there is a lot of flexibility and variability** amongst final formulations.
- Designing an appropriate product necessitates the interpretation of **ill-defined or vague preferences.**
  - What determines a *good* cup of coffee?
  - What determines a *high-quality* cup of coffee?

SCA Standards

- Some standards exist, but are still evaluated in a subjective way.
  - **Flavor:** “midranges”
  - **Acidity:** “fruit/wine”
  - **Body:** “mouthfeel”
  - **Aroma:** “volatility”
  - **Aftertaste:** “finish”
- Helpful, but not common amongst **general audiences.**



Specialty Coffee Association

Specialty Coffee Association
Arabica Cupping Form

Name:
Date:
Table no:

Quality Scale

6.00 - GOOD	7.00 - VERY GOOD	8.00 - EXCELLENT	9.00 - OUTSTANDING
6.25	7.25	8.25	9.25
6.50	7.50	8.50	9.50
6.75	7.75	8.75	9.75

Sample No. | Roast Level of Sample | Fragrance/Aroma Score (Dry, Qualities, Break) | Flavor Score | Acidity Score (Intensity: High, Low) | Body Score (Level: Heavy, Thin) | Uniformity Score | Clean Cup Score | Overall Score | Total Score

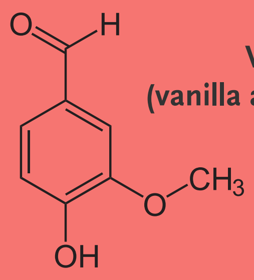
Aftertaste Score | Balance Score | Sweetness Score | Defects (subtract): Taint - 2, Fault - 4, # of cups x intensity =

Notes: | Final Score

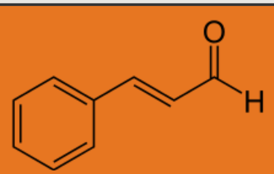
What do People Look For in Coffee?

“Taste, Smell, how efficiently it can be produced, the time it takes to roast the coffee, the effect it has on the person drinking it.”	Flavor metric, odor metric, "efficiency" metric, roasting time, "drinking effect" metric
“On an individual scale, the amount of milk/sugar added”	Quantity of milk, quantity of sugar
“How old the coffee beans are (if too old, have they lost flavor/strength), amount of time spent roasting, conditions that beans were grown in”	Bean age, roasting time, growing location
“I want it to be sourced somewhere that pays ethically. Also that has high caffeine content so that I don't have to drink multiple cups a day and seem crazy. I also like coffee that can be brewed so strongly that it makes my friends gag when they smell it”	Growing location, caffeine concentration, coffee strength
“Making sure the ag practices are sustainable. I would then look at the quality of beans to get a flavor that would taste good.”	Sustainability metric, "quality" metric, flavor metric

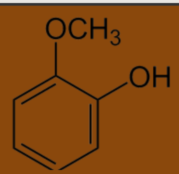
The Coffee Flavor Wheel



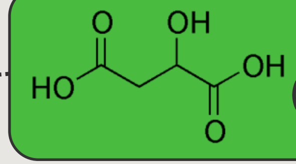
Vannillin
(vanilla and sweetness)



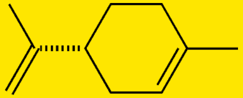
Cinnamaldehyde
(cinnamon and cloves)



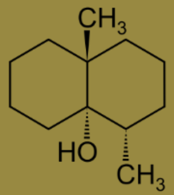
Guaiacol
(wood smoke)



Malic Acid
(apples and stone fruit)



Limonene
(citrus)



Geosmin (earth and wood)

What's Actually In Coffee?

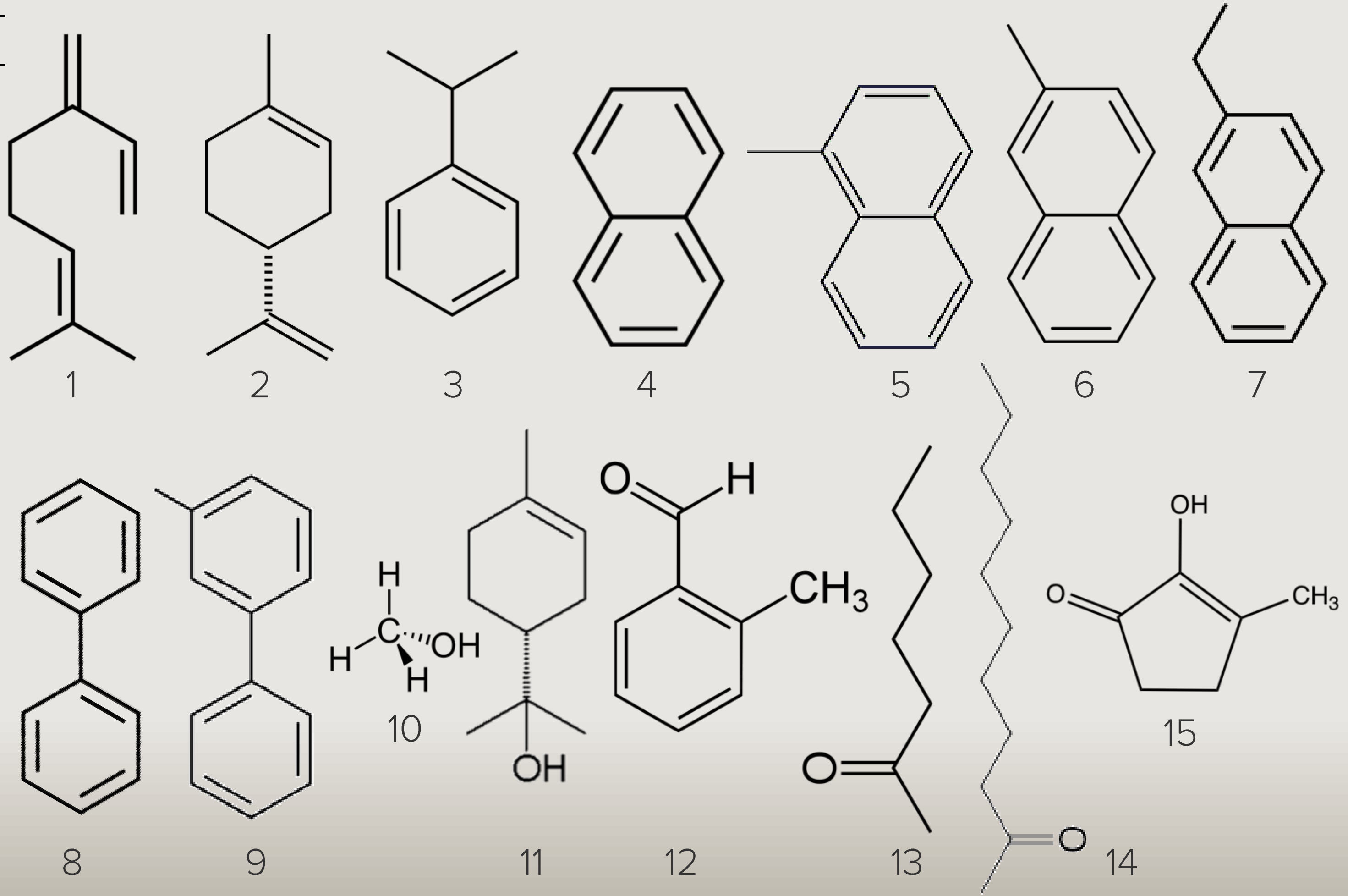
Table 2. List of compounds identified in coffee and typical analytical methods

No.	Compounds	Typical concentration	Comment	Analytical methods	References
1	Chlorogenic acids	0.6-26.4%	More than 10 types of acids	HPLC, LC/MS	Trugo et al., 1984; Clifford, 2000; Mullen et al., 2011
2	Caffeine, theobromine, theophylline	3-350μg/mL		HPLC, LC/MS	Wanyika et al., 2010; Bispo et al., 2002; Eanyika et al, 2010
3	Trigonelline	3-10 mg/g		HPLC, LC/MS	Ky et al., 2001; Casal et al., 2000
4	Carbohydrates	3.41-9.43%	Saccharose, glucose, fructose, arabinose, galactose	IC	Knopp et al., 2006
5	Amino acids	4.4-1075 mg per 100g coffee powder	16 amino acids	IC, HPLC, LC/MS	Nakhmedov et al., 1984; Bytof et al., 2005
6	Vitamins	less than 3mg	Vitamin B_1, riboflavin (B_2), nicotinic acid (PP), pyridoxine (B_6), tocopherol (E), vitamin B_{12}	HPLC	Clarke, 1985; O'Driscoll, 2014
7	γ-aminobutyric acid	30-1860 mg/kg		HPLC	Bytof et al., 2005, Kramer et al., 2010
8	Serotonin	about 10 mg/g dry weight	'happiness hormone'	HPLC	Kele and Ohmacht, 1996
9	Organic acids	about 1%	Citric, malic, oxalic, acetic acids, etc.	HPLC	Kele and Ohmacht, 1996; Mabrok and Deatheroge, 1956
10	Anions	phosphates 0.2%, sulfates 0.1%	Fluoride, chloride, nitrate, sulfate, phosphate	IC	Mabrok and Deatheroge, 1956
11	Oxyaromatic acids	3-6%	Ferulic, n-coumaric, 3,4-dimethoxycinnamic, 3,4,5-trimethoxycinnamic, sinapic acids	HPLC	Clarke, 1985; Clifford, 2000; Murata et al., 1995
12	Tannins	3.6-7.7%		Spectrophotometry	Clarke, 1985; Savolainen, 1992
13	Polysaccharides	over 12%	Cellulose, pectic substances, fibers	IC, HPLC	Clarke, 1985; Moreira et al., 2012
14	Melanoidins	5-60 g/100g	Dark brown natural coloring agent	HPLC, DPPH assay	Clarke, 1985; Moreira et al., 2012; Pérez-Hernández et al., 2012
15	Mineral substances	3-4.5%	Potassium, magnesium, calcium, sodium, iron, manganese, zinc, copper	ICP/MS	Clarke, 1985; Abdulmadjid et al., 2017

- One can gain some insight on the relevant flavor markers of coffee through the same analytical techniques we use in other engineering applications.
- Minor caveat: **absolute concentration does not directly correlate with the perception of flavor.**

What’s Actually In Coffee?

No.	Compounds
1.	β-myrcene
2.	limonene
3.	n-cumene
4.	naphthalene
5.	1-methylnaphthalene
6.	2-methylnaphthalene
7.	2-ethylnaphthalene
8.	biphenyl
9.	3-methylbiphenyl
10.	methylol
11.	α-terpineol
12.	2-methylbenzaldehyde
13.	2-heptanone
14.	2-undecanone
15.	3-methyl-2-hydroxy-2-cyclo-pentane-1-one



Coffee Chromatograms

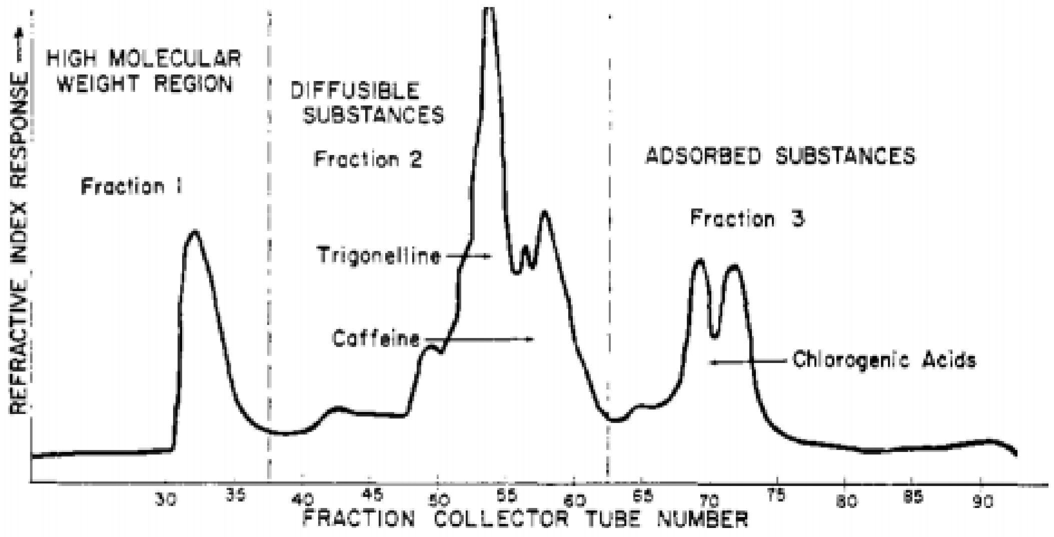


Figure 3. Chromatographic separation of roasted Santos coffee water extract on Sephadex G-25 column

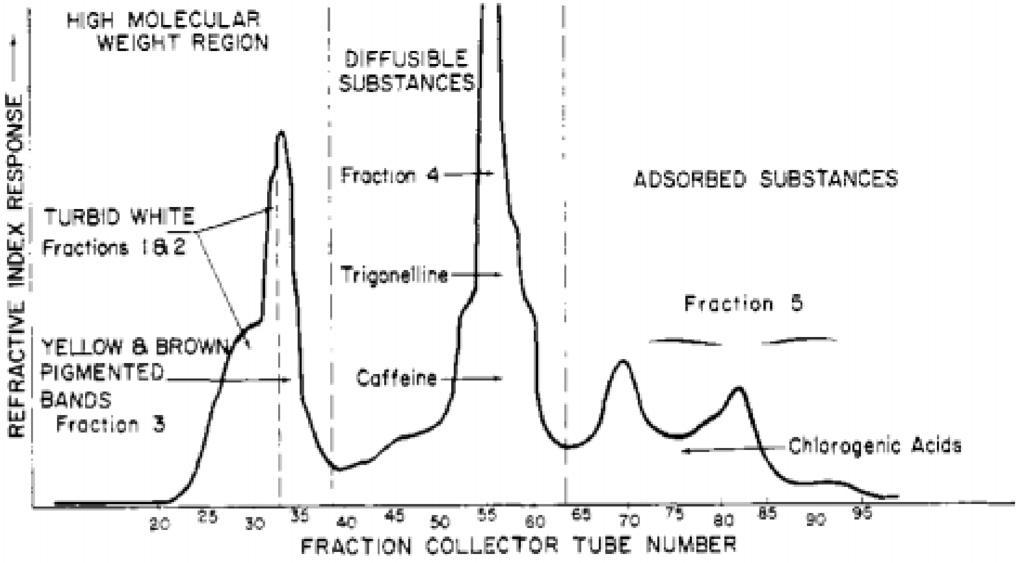
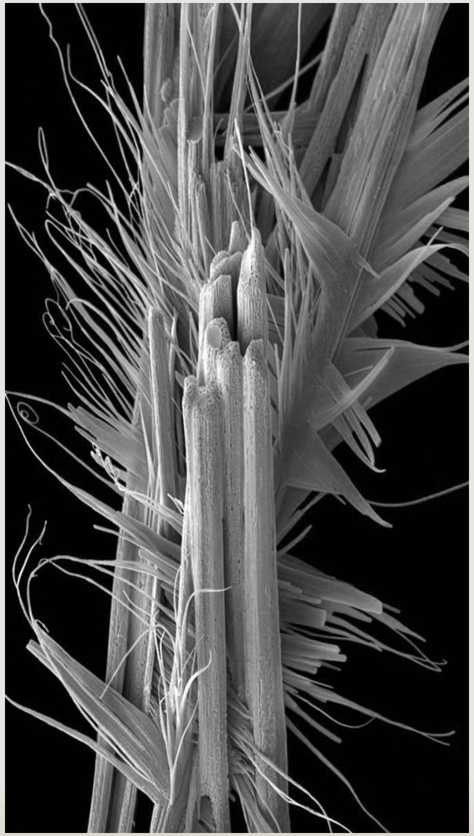


Figure 4. Chromatographic separation of green Santos coffee water extract on Sephadex G-25 column

Unsurprisingly, the extent of roast also changes the prevailing organic profile.

A Minor Aside - Caffeine



- Arguably, the compound that coffee is most designed or engineered around is not deeply considered in the tasting process!
  - Caffeine does in fact have a flavor – in fact, it is defined by some as a **prototypical bitter.**
  - **Approx 100-200mg/250mL coffee, or 50-75mg/30mL espresso.**
- Caffeine has a half-life of 1.5-9.5 hours, but like any stimulant will have dosage effects that can vary from person to person.

The Question

W.B. Sunarharum et al. / Food Research International 62 (2014) 315–325

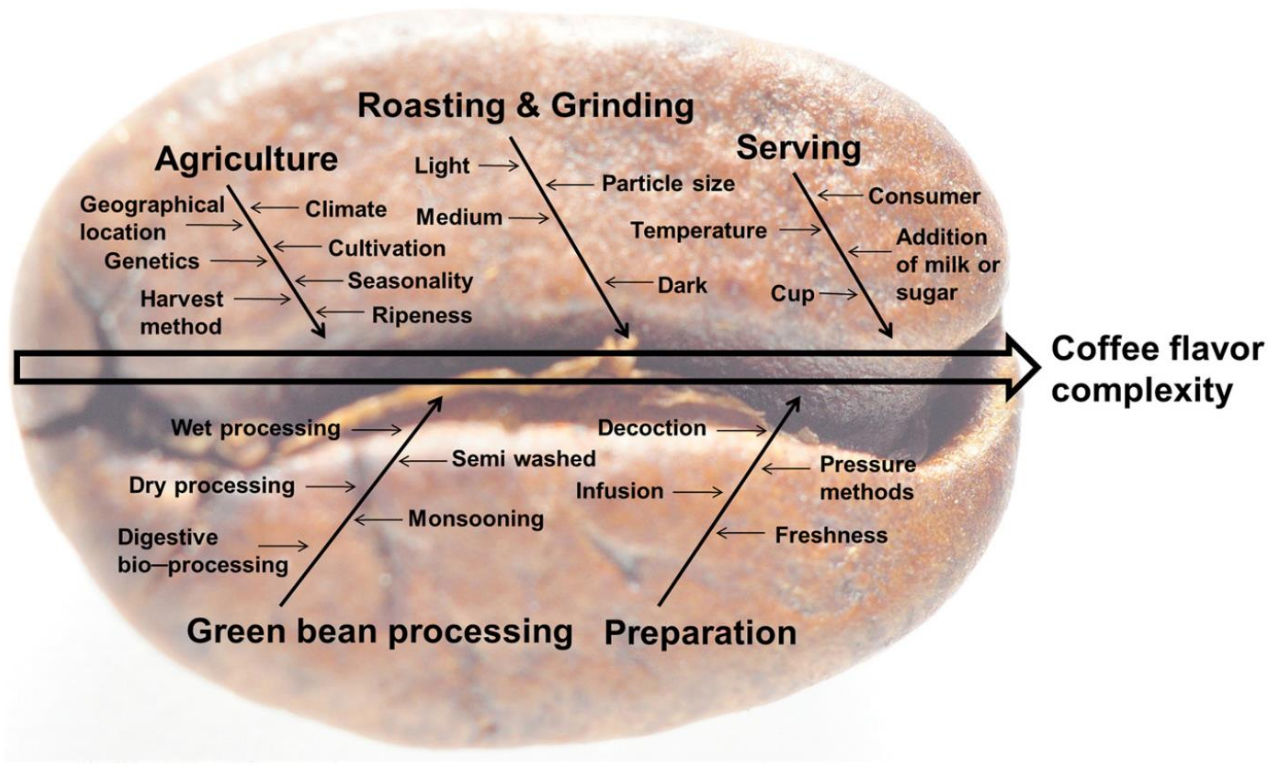


Fig. 1. Factors that influence coffee flavor complexity from farm to cup.

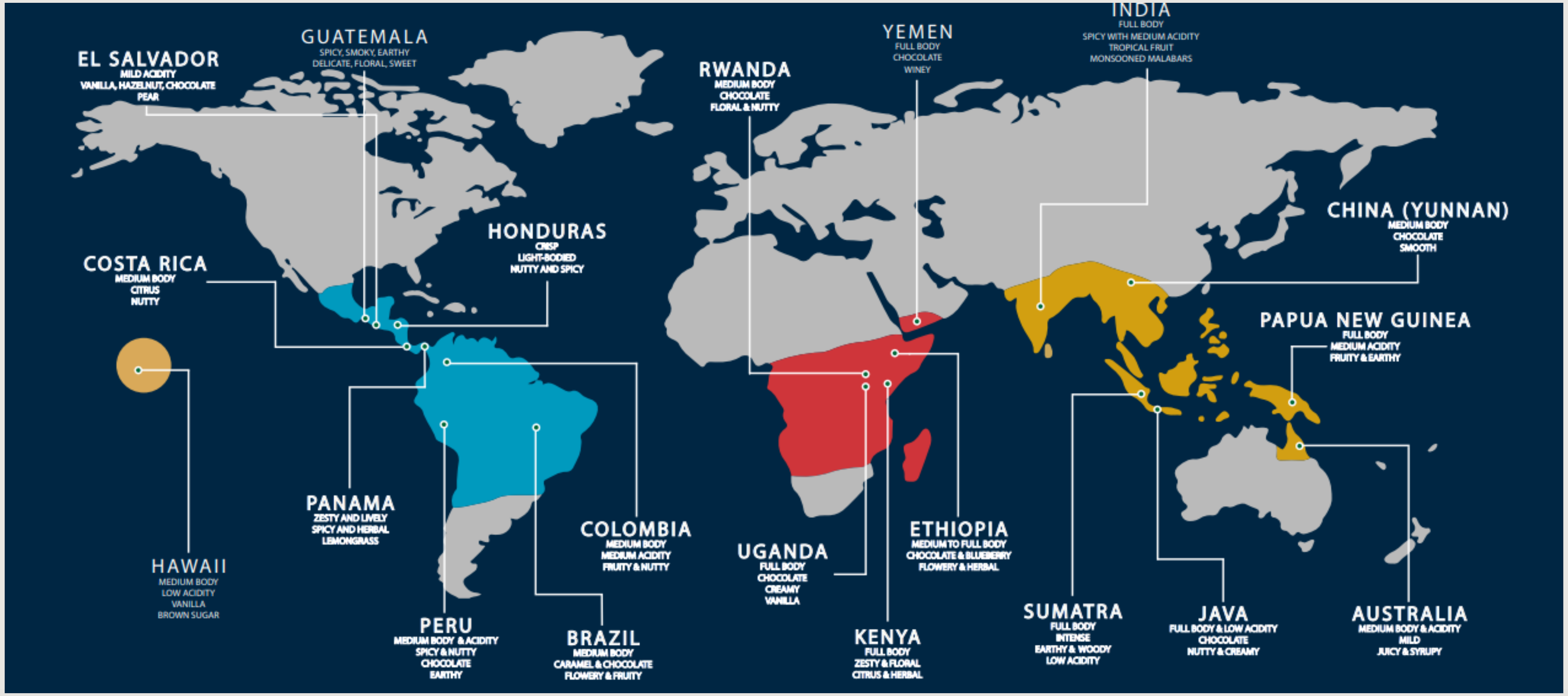
- As engineers, **how can we use our skills to achieve the flavors and experiences we are aiming for?**
- How can we use our knowledge of chemical engineering to ensure robustness and control under many conditions?

The Starting Materials – Bean Sourcing

Coffee originates from **Ethiopia** – and requires ambient conditions comparable to this location.

- Indirect but **bright sunlight**
- Relatively **high humidity**
- **Moist** but not waterlogged soil
- Temperatures **above 18°C** (65°F) but also limited periods of high temperature.

Different locations yield similar, but distinct flavor profiles owing to local soil chemistry.

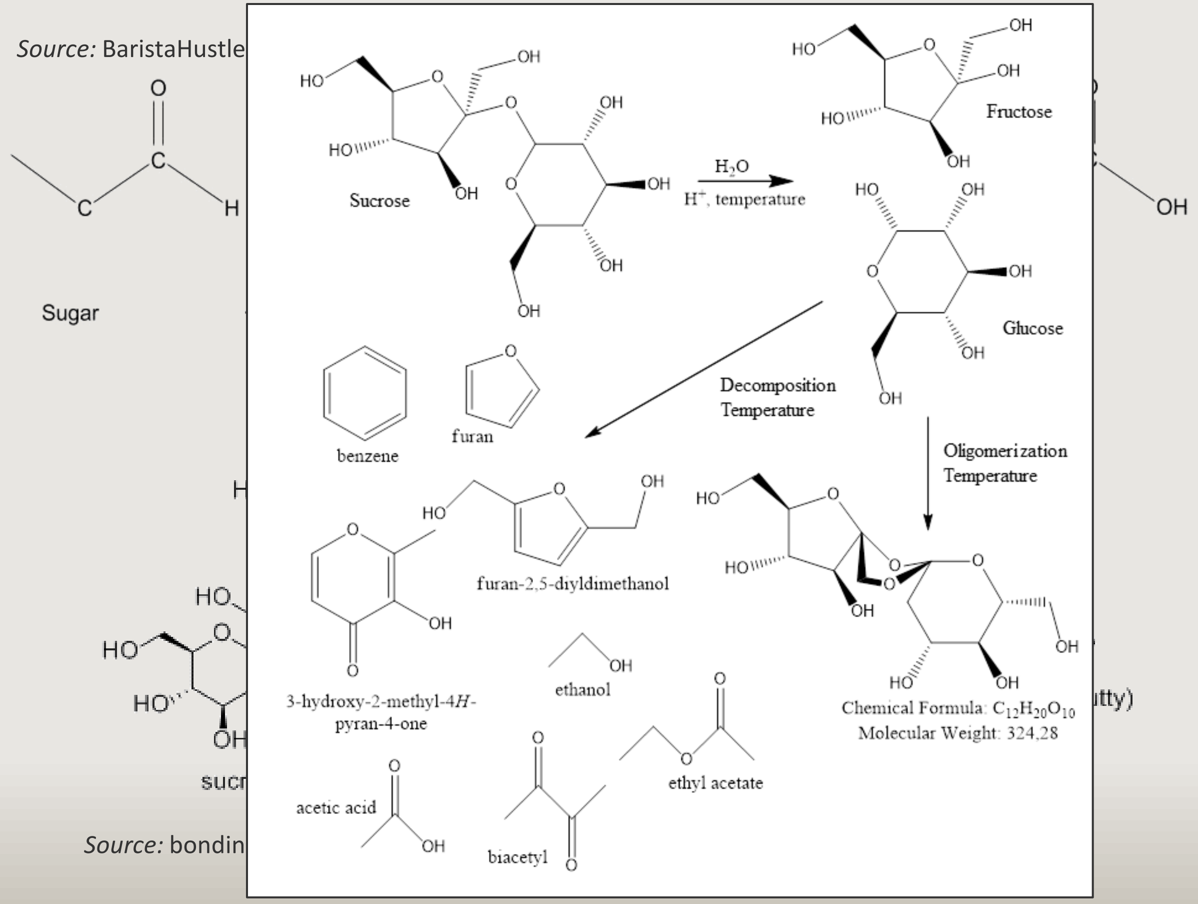


Roasting Coffee

- As it is roasted, coffee takes on **many different scents, flavors, and appearances.**
- Rate of heating
- Final temperature dictates the “level” of roast:
  - 180°C – “Blonde roasts”
  - 200°C – “Medium roasts”
  - 225°C – “Dark roasts”

Parallel Roasting Chemistry

- **Maillard Reactions** (140°-170°C)
- **Caramelization** (150°-180°C)
- **Pyrolysis** (180°C+)
- Throughout this process, **water and CO_2 are liberated,** yielding the “cracks” heard throughout roasting.



Roasting Mechanics

- Objective: roast **uniformly and quickly.**
- Beans will absorb ambient energy through **Newton's Law of Cooling** (or in this case, Heating):

$$Q = hA(T_{bean} - T_{env})$$

$$T_{bean} = T_{env} + \left(T_{bean,0} - T_{env}\right)e^{-rt}$$

- If the heat transfer coefficient, h, is too small, the relative importance of internal heat transfer increases – resulting in **uneven roasting.**

$$Bi = \frac{h\left(\frac{V_{bean}}{A_{bean}}\right)}{k_{bean}}$$

Drum Roasters

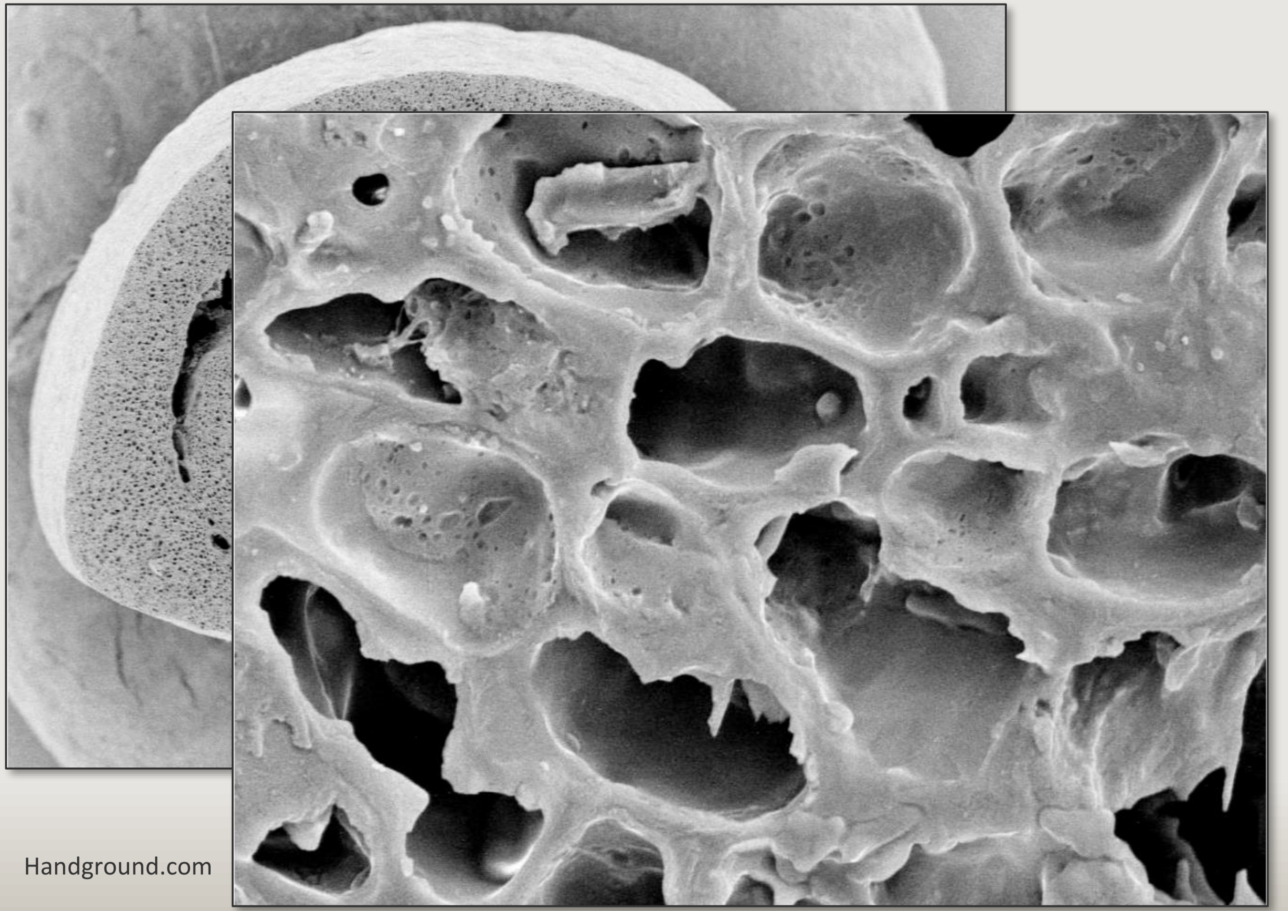
- Traditional drum roasters **slowly rotate beans near a heating element to promote mixing.**
- Batch production introduces scalability issues – while roasters can be made arbitrarily large, **beans are going to be the same size.**

Heated Fluidized Beds

- Chemical engineer Michael Sivetz noted similarities in the **functional purpose** of a heated magnesium pellet dryer – using **convection to enhance heat transfer through the continuous throughput of air.**
- Forced convection leads to faster throughput of roasting (6-10 minutes vs. 15-20 minutes.)
- Convection also results in **mass** loss compared to drum roasting – leading to differences in drying rates and loss of volatiles.

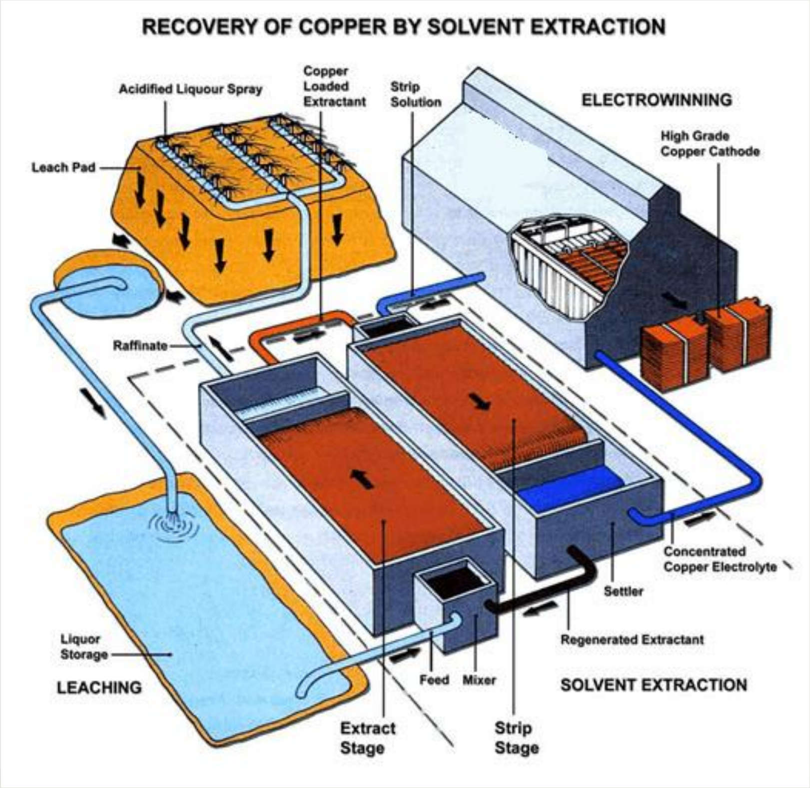
Preparing Coffee

- **Roughly 30% of a coffee bean's mass is soluble**, and not every compound is something that will necessarily taste good. Some are structurally similar to each other.
- After roasting, how can we expose coffee to water such that **only desired flavors are achieved?**



Handground.com

Solid-Liquid Leaching



- The overall principle is nearly identical to industrial applications for industrial solid-liquid leaching!
- In all applications, **a solid substrate is ground to a high-surface media for improved dissolution of a desired product.**
- Factors for Extraction:
  - **Size and porosity** of solid particles
  - **Extraction state** (pressure, temperature)
  - **Solvent** properties and composition

Common Means of Extraction: Pour-over

- Hot water is poured over **medium/coarse-ground** beans, around 18:1 water/bean ratio.
- **Slow** (3-5 minutes), **low-pressure,** non-continuous exposure to beans
- Paper filter blocks many oils/solids, resulting in a “cleaner” cup.

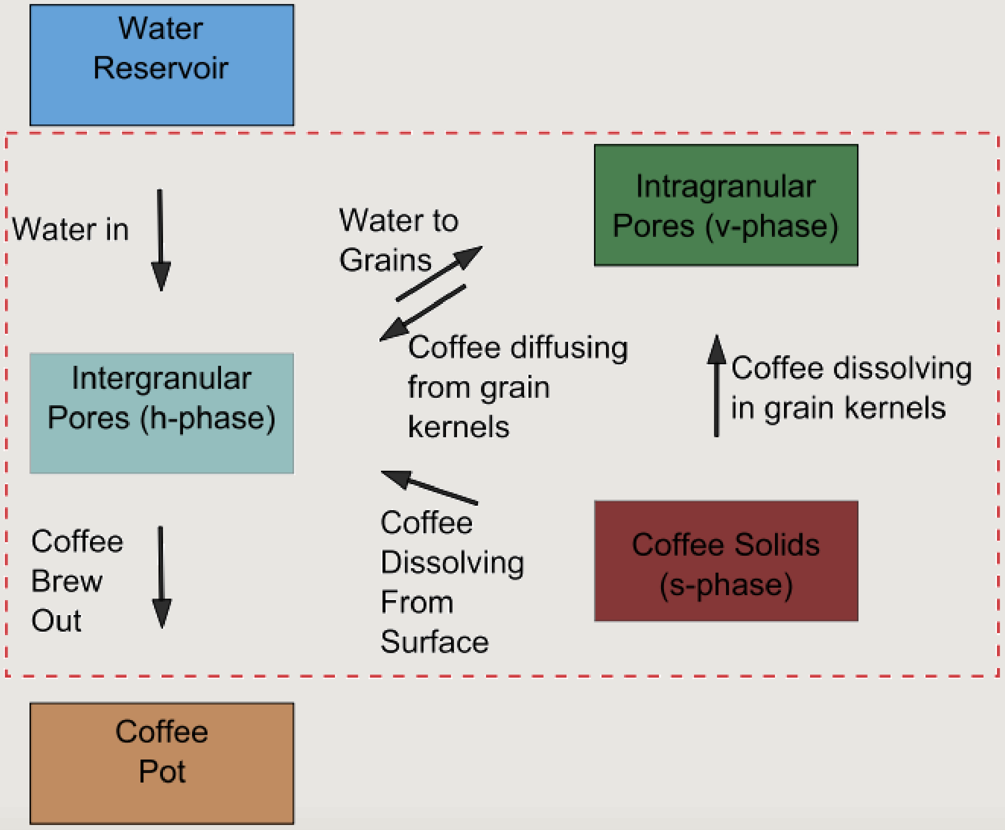
Common Means of Extraction: French Press

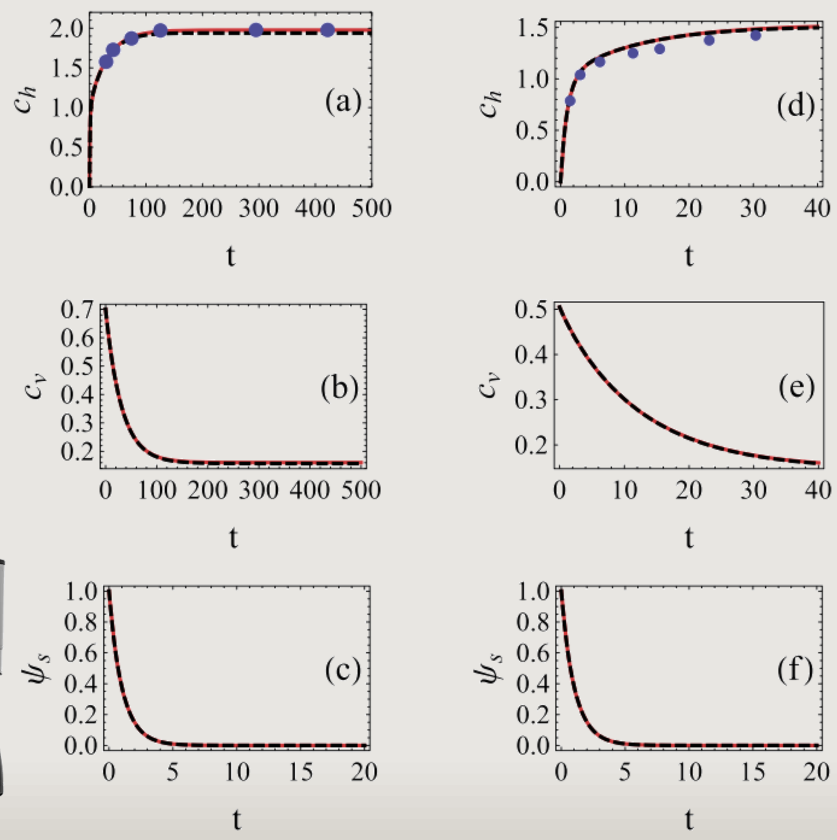
- Hot water is mixed into **coarsely-ground beans** and pushed aside using a metal filter, around 15:1 water/bean ratio.
- **Slow** (3 min), **batch-wise**, **low-pressure** continuous exposure to beans
- Metal filter allows passage of oils, fine solids, increasing cup body.

Common Means of Extraction: Espresso

- Hot water is pushed through finely ground beans that have been packed into a pressurized metal filter, around **1.5:1 water/bean** ratio.
- **Fast (30 seconds), high-pressure** continuous exposure to beans
- Metal filter allows for passage of oils and very fine solids. The pressure yields a *crema* on a properly prepared espresso.

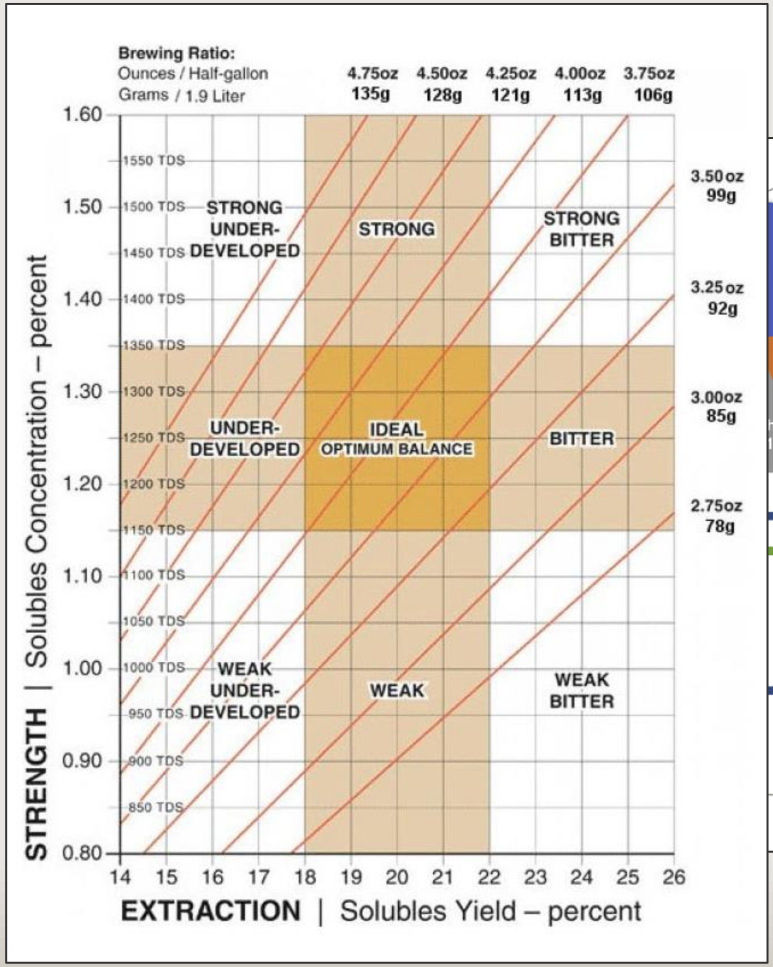
Models for Extraction

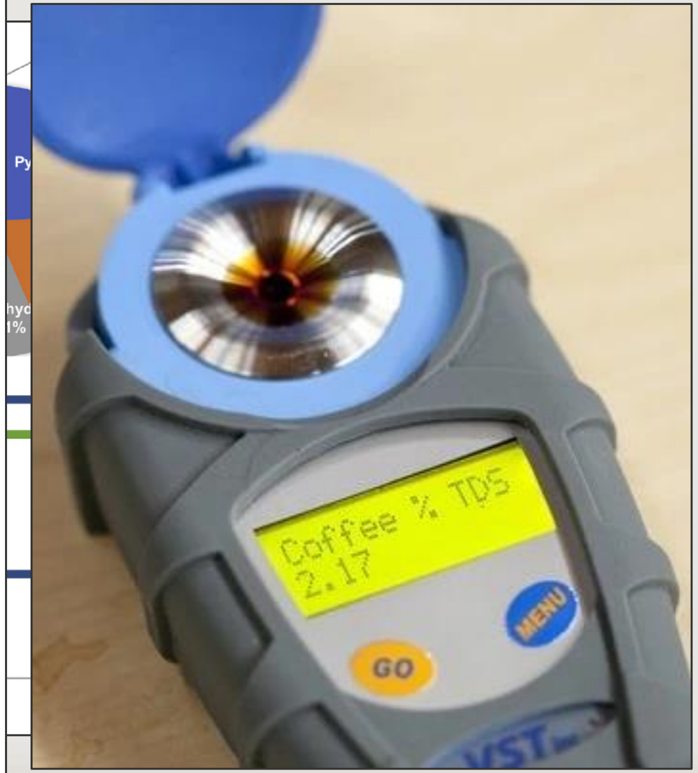




Non-Uniform Extraction

- Like in **chromatography**, different compounds will pass through at different rates – yielding changes in flavor characteristics.
- **One cannot compensate for using too little beans by extracting for longer periods of time!**



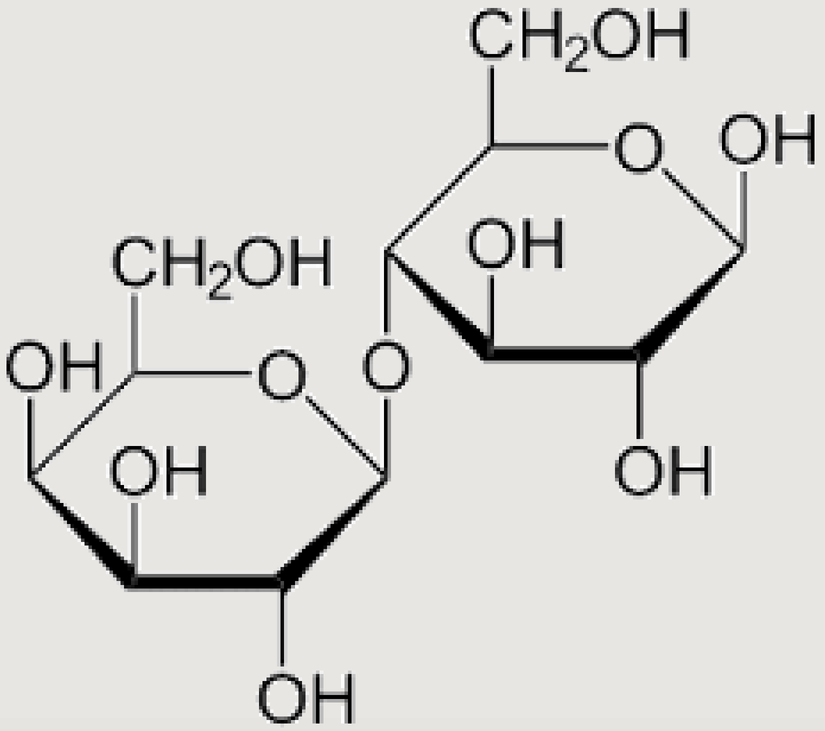


Further Modification – Adding Extra Ingredients

- Just as common as the actual extraction of coffee is the **personalization of coffee** – at its core, this is chemical engineering at its finest!
- From the consumer end, additives are one of the main ways in which flavor and experience can be adjusted.
  - Amplify/attenuate existing flavor perception
  - Add otherwise non-existent properties

Sugars

- A significant source of **calories** if added to coffee. Can also arise from steamed milk.
- While sugar in very high quantities can adjust viscosity and texture, this is seldom enough to adjust overall drink properties.
- So, its primary purpose is usually to mask or drown out other taste percepts (i.e. bitterness.)



Milk

Starbucks uses more than 100 million gallons of milk on an annual basis. By design, milk is **calorie dense** and contains a variety of nutritionally relevant components!

- 87.7% Water
- 5% Lactose
- 3.4% Fat
- 3.3% Proteins
- 0.7% Minerals

Milk and Flavor Perception

Table 1—Sweetness intensity[a] and persistence times[b] and flavor intensities of sucrose-sweetened drinking chocolate containing surfactants (mean values of 14 panellists)

% Surface active agent in drinking chocolate solution	Sweetness				Flavor[c]	
	Lecithin		GMS		Lecithin	GMS
	Intensity score	Persistence time (sec)	Intensity score	Persistence time (sec)	Intensity score	Intensity score
0.2	4.6	15.4	5.5	16.6	6.0	6.1
0.4	4.8	16.8	5.6	18.7	5.7	5.9
0.6	4.9	17.1	5.8	21.4	5.3	5.6
0.8	5.0	17.3	5.9	22.2	5.1	5.5

Anova tests for significance:

[a] Sweetness intensities significantly different ($p < 0.001$) from one concentration to next of each surfactant; also significance between surfactants ($p < 0.001$).

[b] Persistence times significant from one concentration to next of each surfactant ($p < 0.05$) and between surfactants ($p < 0.001$).

[c] Flavor scores significantly different between concentrations of surfactant ($p < 0.001$) and between surfactants ($p < 0.01$).

Milk and Flavor Perception

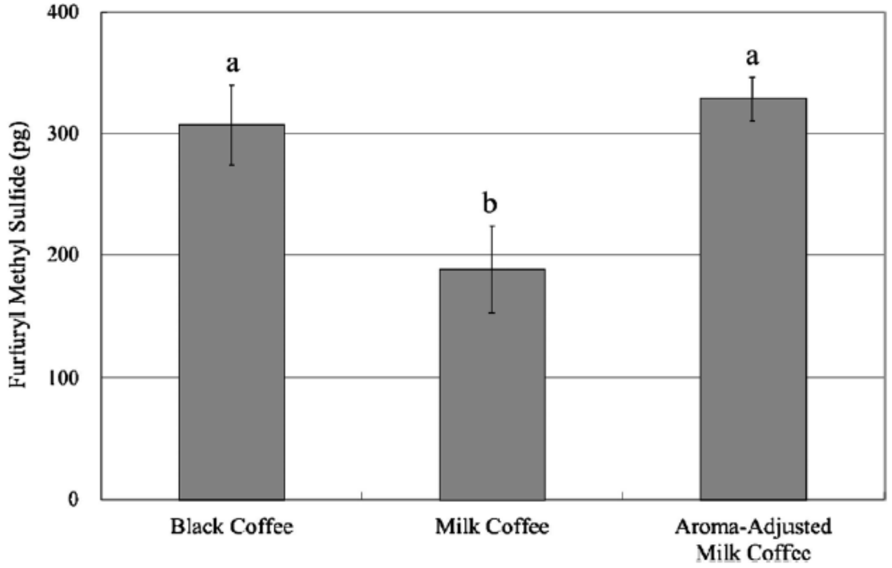


Fig. 1. Semiquantitative amounts of furfuryl methyl sulfide (FMS) exhaled through the nostrils during the consumption of black coffee, milk coffee, and aroma-adjusted milk coffee. Each amount of FMS is the mean value of triplicate results obtained from one panelist. Error bars show the standard deviations and the letters a and b indicate means that significantly differ at $p < 0.01$ (Tukey's test).

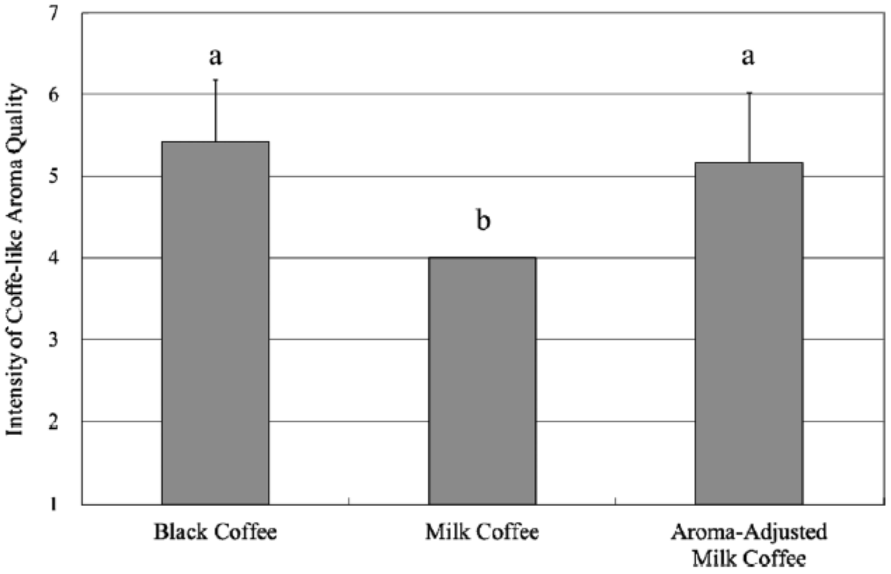
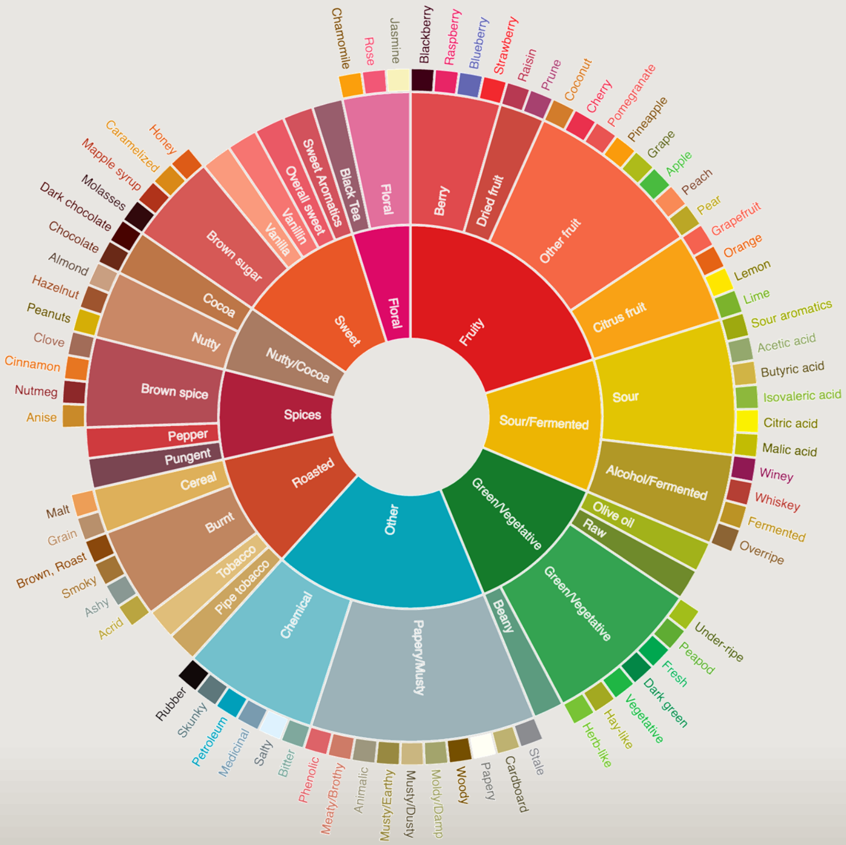


Fig. 2. Intensity of coffee-like aroma quality during the consumption of black coffee, milk coffee (control, the intensity was defined as 4), and aroma-adjusted milk coffee. Each intensity is the mean value of 31 panelists using a seven-point scale from 1 to 7. Error bars show the standard deviations and the letters a and b indicate means that significantly differ at $p < 0.01$ (Tukey's test).

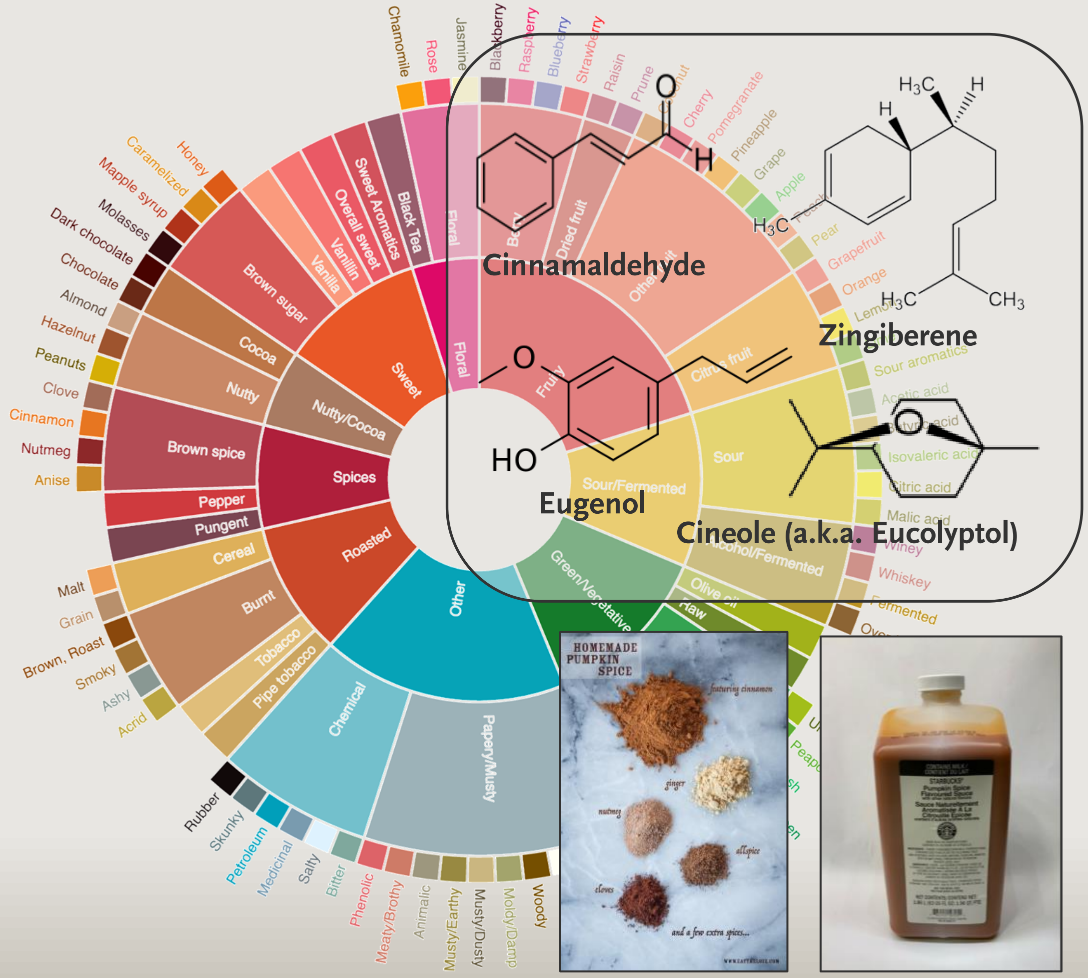
"The present results suggested that the significantly decreased intensity of the coffee-like aroma quality might result from decreased aroma release of a few odorants, including 2-furfylthiol, by the addition of milk to the coffee."

More Creative Additives

- Consider some of **Starbucks' most popular coffee beverages.**
  - **Mocha** Frappuccino
  - Iced **Caramel** Cloud Macchiato
  - **(Vanilla) Sweet Cream** Nitro Cold Brew
  - **Vanilla Bean** Crème Frappuccino
  - **Honey** Flat White
  - Salted **Caramel** Mocha Coffee Frappuccino
  - **Pumpkin Spice** Latte
- These flavors (unsurprisingly) show up in the Coffee Flavor Wheel!



What's Actually in Pumpkin Spice?



- Actual Pumpkin Spice (as in, the spice added to make pumpkin pie):
  - 18g Cinnamon → Cinnamaldehyde
  - 4g Nutmeg → Sabinene
  - 4g Ginger → Zingiberene
  - 3g Cloves → Eugenol
  - 3g Allspice → Eugenol, Cineole, Caryophyllene
- A mixture of the main **character impact compounds** are used to evoke the flavor of pumpkin spice.

Flavor Adulterants

- Knowing some of the identifying features and/or dominant flavor notes means that one can emulate expensive products with **significant markup.**
- Coffee is no exception – **premium** flavors and consistencies have been copied through the addition of other materials!

Other Design Considerations

- Flavor is an **important** factor in determining product design, but is often not the only constraint.
  - **Time** for preparation
  - Shelf **stability** of product
  - **Choice/flexibility** of operation
- Chemical engineers see this as an opportunity to **optimize and automate.**

Case Study: Keurig

- The K-Cup single serve coffee pod addressed many of these issues, though introduced others in its place.
- Pros:
  - Instant (<2 minute) fresh coffee
  - Full automation of brew process
  - Large selection
- Cons:
  - Inconsistent product ecosystem and model incompatibilities
  - Environmental footprint
  - Physical space density

Case Study: Keurig Alternatives

Senseo Pods

Flavia Filterpacks

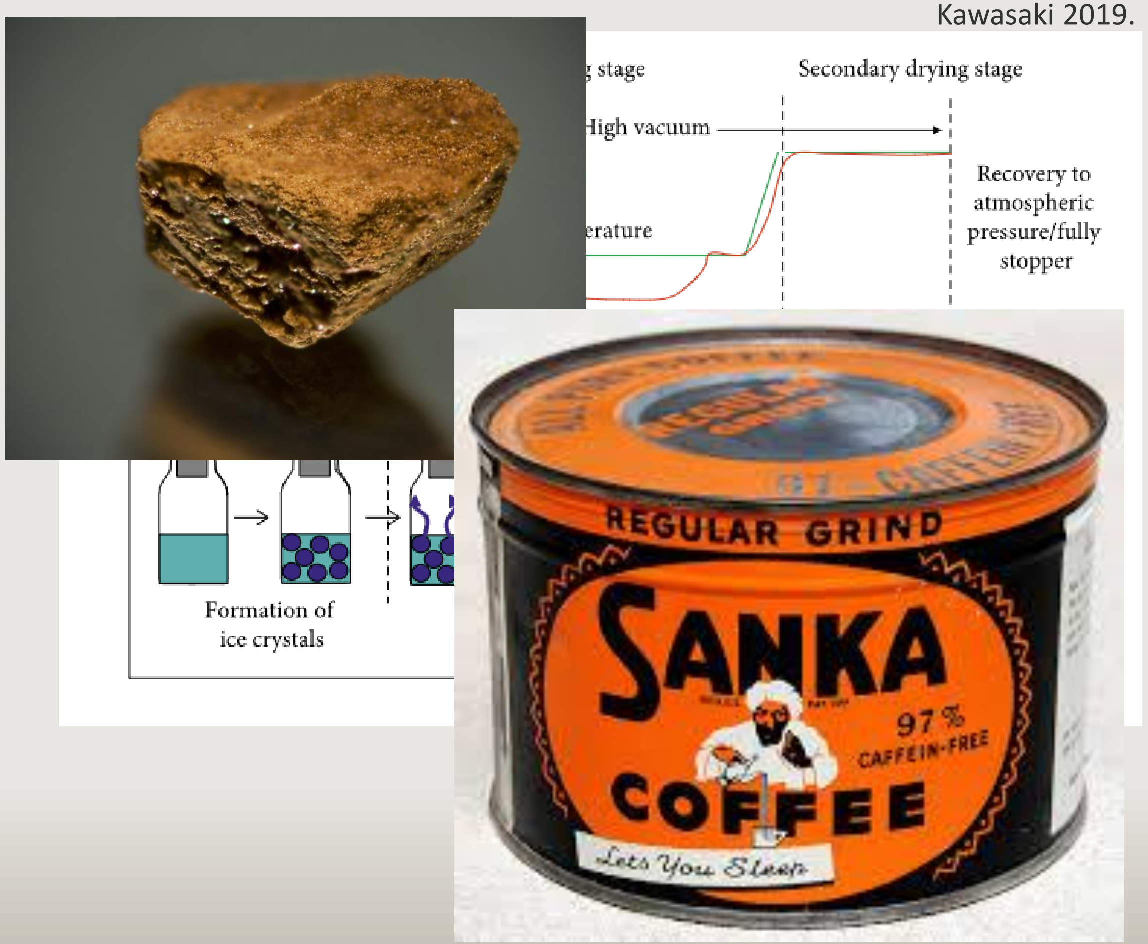
Tassimo T-Discs

Nespresso Capsules

Case Study: Instant Coffee

- Older technologies utilized **lyophilization** or **spray-drying** processes, focusing on the soluble coffee components over the grounds themselves.
- Pros:
  - High space density per cup
  - Shelf stable for long periods
- Cons:
  - Loss of volatiles/solubles in drying process

Kawasaki 2019.



Conclusions

- In practice, **there is no silver-bullet solution to the production of a "perfect cup" of coffee, as design constraints and will result in contextually optimal solutions.**
- Chemical reactions and mass transfer phenomena dictate the amounts of flavor compounds that wind up in a final product.
- Post-processing introduces additional flexibility and design space for individual users.
- For your own cup, **you are the final decision point!** Drink what makes you happy.