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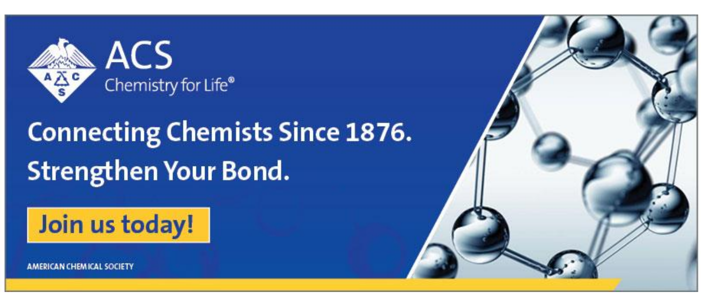

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http://bit.ly/CloudyBeerVideo

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John Esker, Ph.D.
Project Officer – BARDA, U.S. Dept. HHS
ACS Member for 31 years strong!

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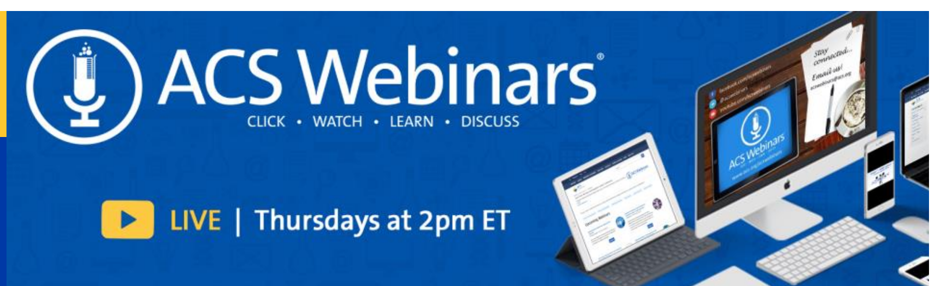

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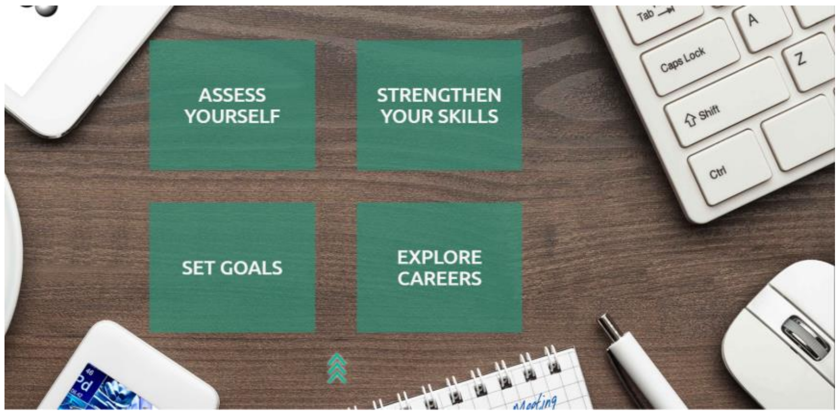

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#HeroesofChemistry
ACS Heroes of Chemistry Award

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Heroes of Chemistry winner BMS: Carl Decicco presenting the story behind Daklinza® and Sunvepra™

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Deadline: Friday, Feb. 1, 2019

2018 Winners: AstraZeneca DUPONT Pfizer SeattleGenetics

www.acs.org/heroes

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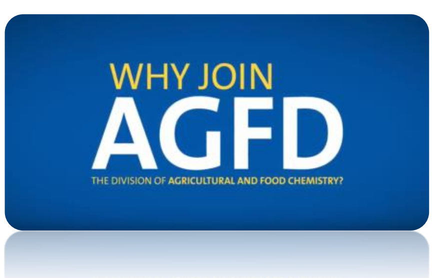
ACS Division of Agricultural & Food Chemistry

ACS Technical Division
Agricultural & Food Chemistry (AGFD)



AGFD brings together persons particularly interested in the chemistry of agricultural and food products, both raw and finished; to foster programs of general papers and symposia on special topics dealing with this field of chemistry; to promote such other activities as will stimulate activity in and emphasize the importance of research in agricultural and food chemistry.

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AGFD Member News: https://agfd.sites.acs.org/agfdmembernews.htm
AGFD Application for Membership: https://agfd.sites.acs.org/agfdapplication.htm

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Upcoming ACS Webinars
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Thursday, November 29, 2018 @ 2-3pm EST

Human Exosomes: *An Ideal Vehicle for Delivery of Therapeutic RNAs to Cells and Organs*

Co-produced with the ACS Division of Medicinal Chemistry and the American Association of Pharmaceutical Scientists

Experts

Hadi Valadi
University of Gothenburg

Alexander Kapustin
AstraZeneca

Tuesday, December 4, 2018 @ 1-2pm EST

Predicting the Biggest Chemistry Advances of 2019

Co-produced with Chemical & Engineering News

Experts

Marshall Brennan
ChemRxiv

Lauren Wolf
Chemical & Engineering News

Claire Hansell
Nature

Michael Torrice
Chemical & Engineering News

Jake Yeston
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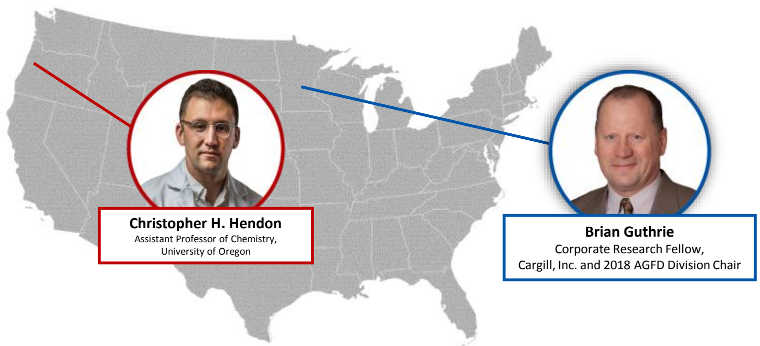
Coffee: *A Chemical and Physical Perspective*



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COHOP COLLABORATION

Hendon Materials Simulation

Coffee

A Chemical and Physical Perspective

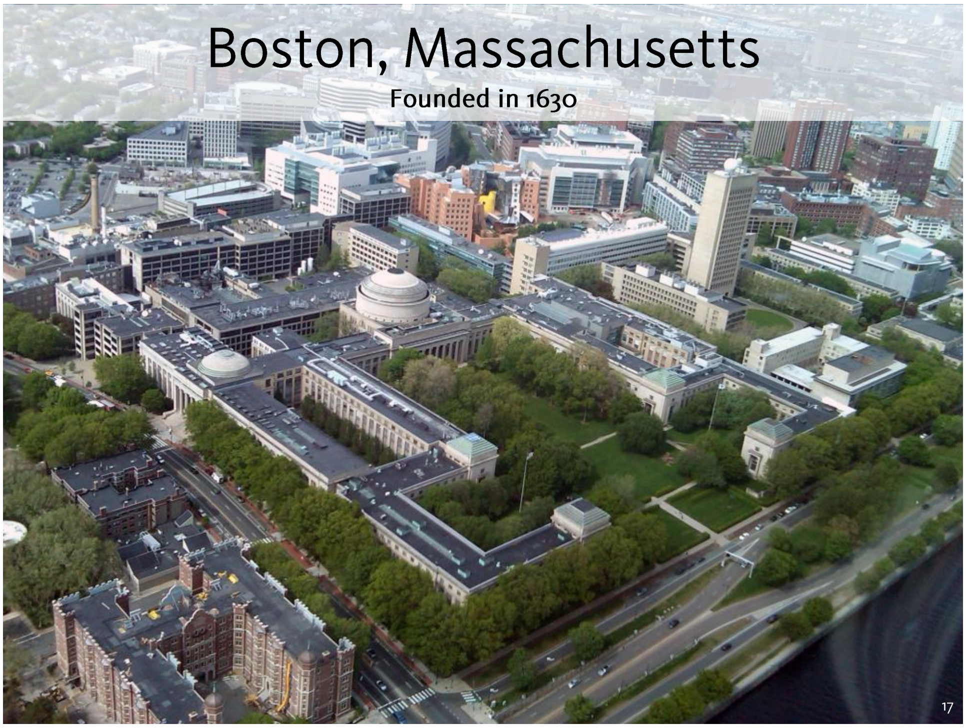
Christopher H. Hendon
Assistant Professor of Chemistry
World Coffee Leader 2016

w: pages.uoregon.edu/chendon
e: chendon@uoregon.edu
t: @chhendon

Coffee literature available at **goo.gl/ Z 1 t X z x**


Bath, United Kingdom
Founded in 3
15


The Roman Baths
16


Boston, Massachusetts
Founded in 1630
17

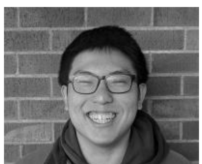

Hendon
Materials
Simulation
Eugene, Oregon
Founded in 1846
18

Hendon Materials Simulation

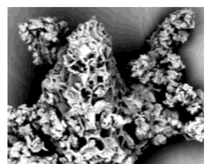
Jenna L. Mancuso
Electro-MOFs
Heterogeneous catalysis

Austin Mroz
Computer-aided learning
Materials discovery

Tom W. Kasel
Photovoltaics
Defective semiconductors



Min Chieh Yang
Molecular redox
Materials assembly

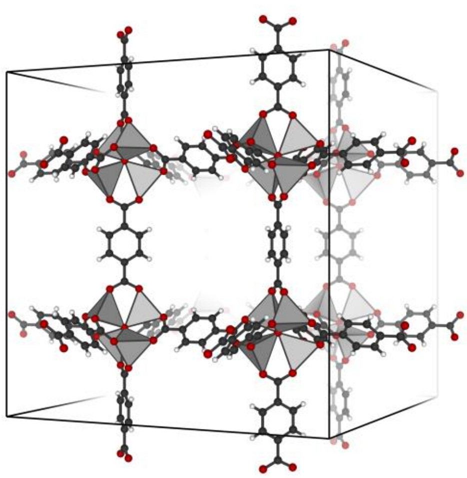


Coffee-related projects

C. Chase Callahan
Metal carbides
Surface catalysis

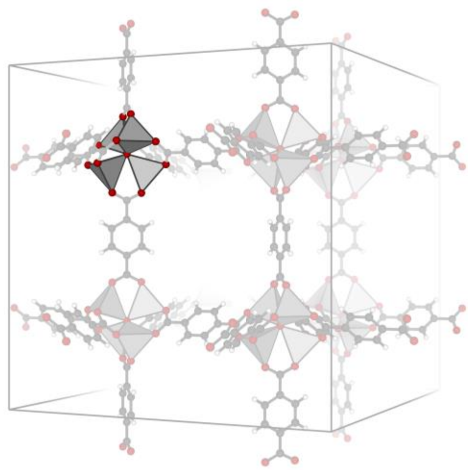
Metal-organic frameworks

A class of porous materials for energy storage and conversion



Metal-organic frameworks

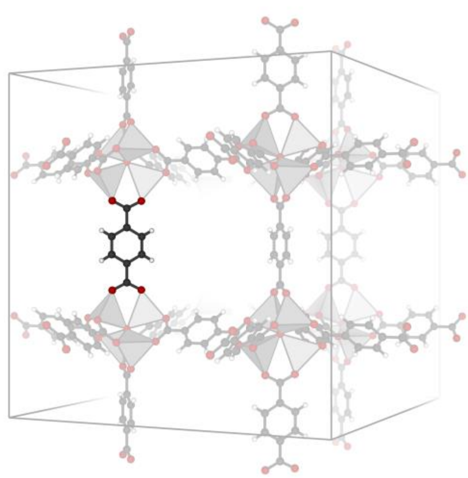
MOFs contain metal-clusters



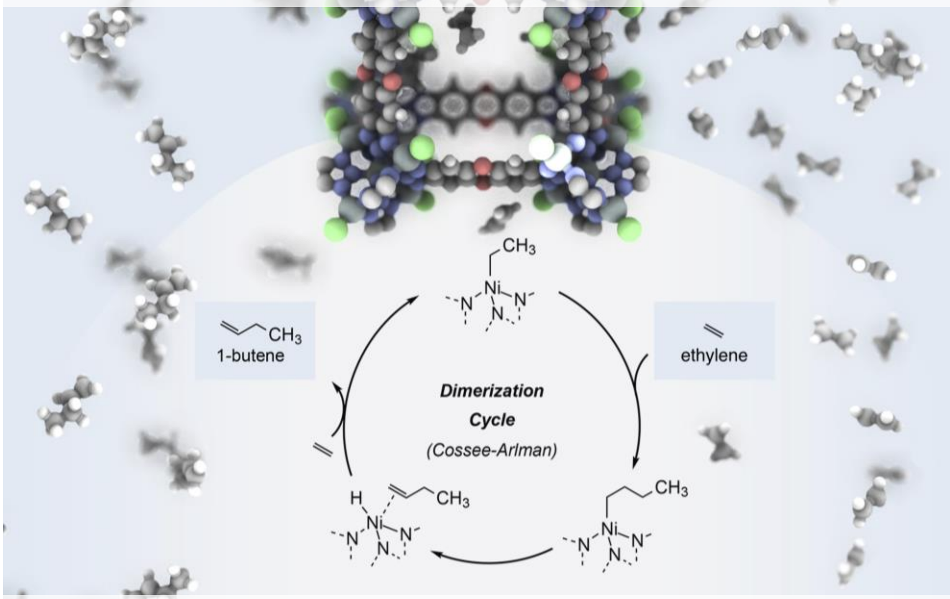
Hendon Materials Simulation

Metal-organic frameworks

Linked together by organic linkers



Single-site heterogeneous catalysis of olefins to their oligomers



ACS Cent. Sci., **2016**, *2*, 148 *J. Am. Chem. Soc.*, **2017**, *139*, 757 *Organometallics*, **2017**, *36*, 1681

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Audience Challenge Question

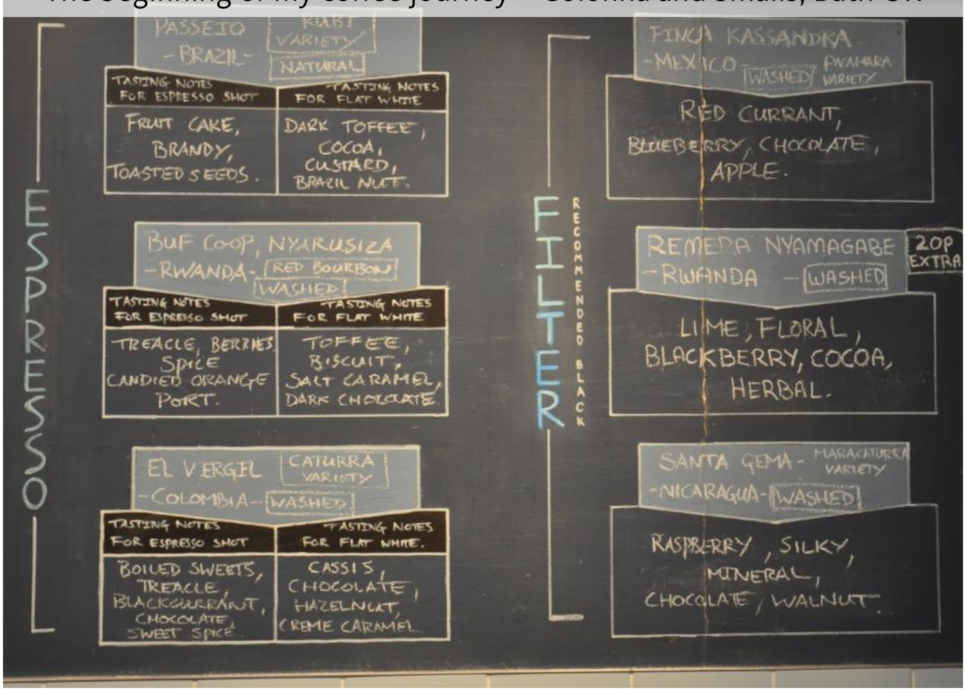
ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT

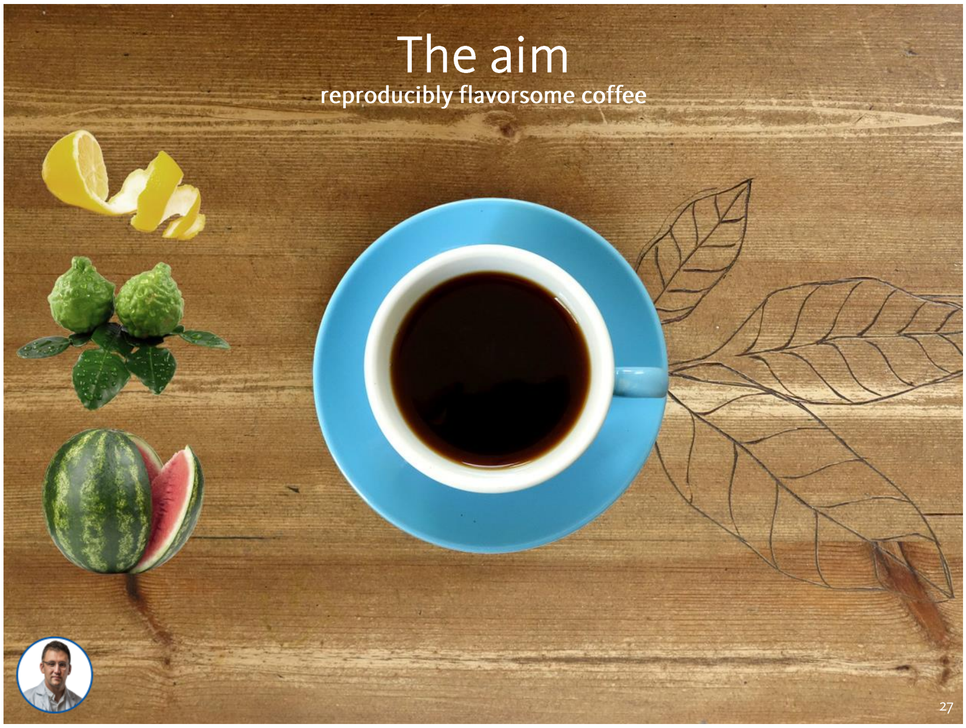
In what field do you work?

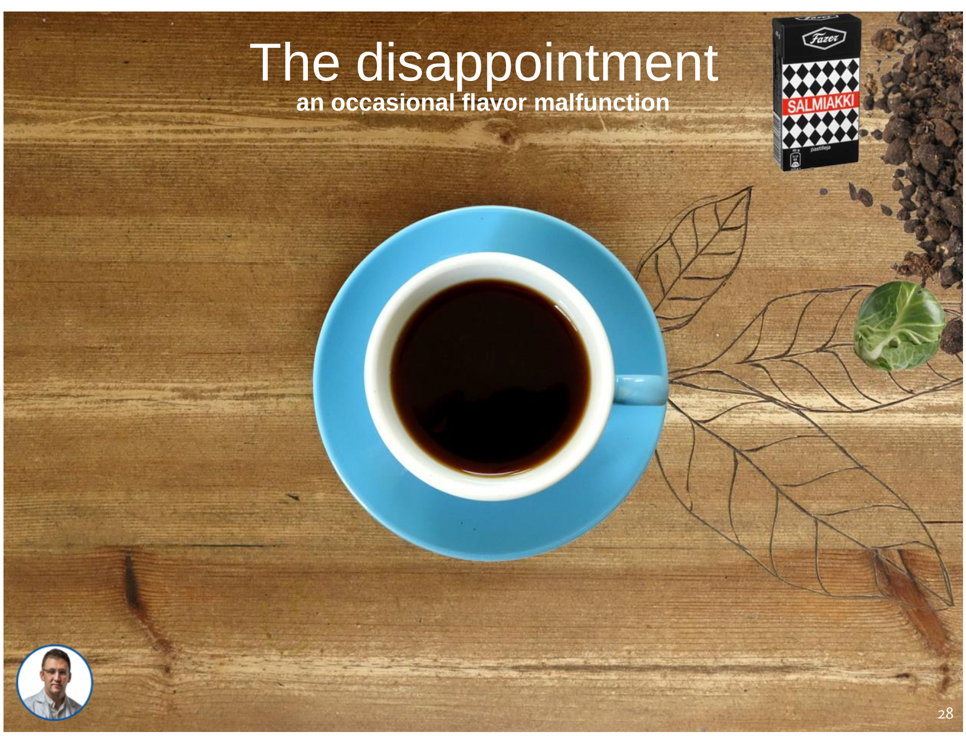
- Coffee Industry
- Chemical Industry
- Academia
- Government
- Other

25

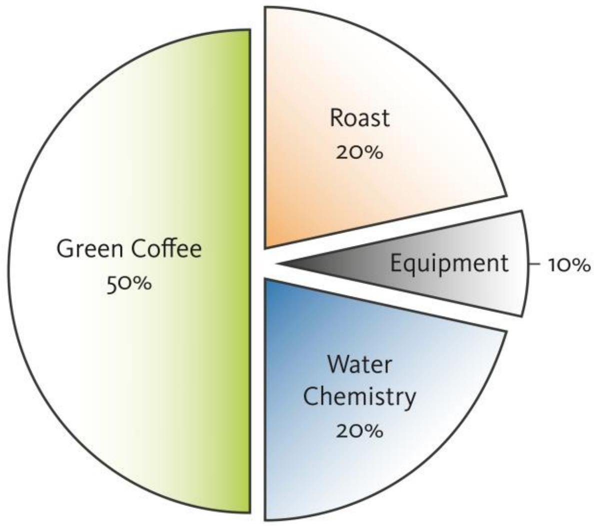
The beginning of my coffee journey – Colonna and Smalls, Bath UK




The aim
reproducibly flavorsome coffee
27

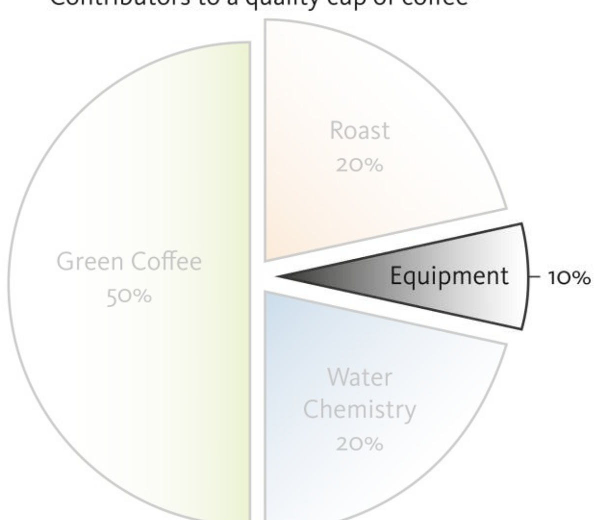

The disappointment
an occasional flavor malfunction
Fazer
SALMIAKKI
28

Contributors to a quality cup of coffee*



* Of course something could go wrong at every stage of brewing.
This figure is rather used to emphasize that quality coffee is less dependent on the brew method.

Contributors to a quality cup of coffee*



* Of course something could go wrong at every stage of brewing.
This figure is rather used to emphasize that quality coffee is less dependent on the brew method.

Coffee is graded on the cupping table

No equipment, just water, coffee coarsely ground, and a spoon + 4 min brew time

Agriculture and Economics

Coffee market analysis

1.3% of USA GDP ($225.2B in 2015)

"Drip" (i.e. filter) coffee dominates the USA

Drip is 1.2 – 1.5 % w/w

Espresso-based beverages prolific in Europe

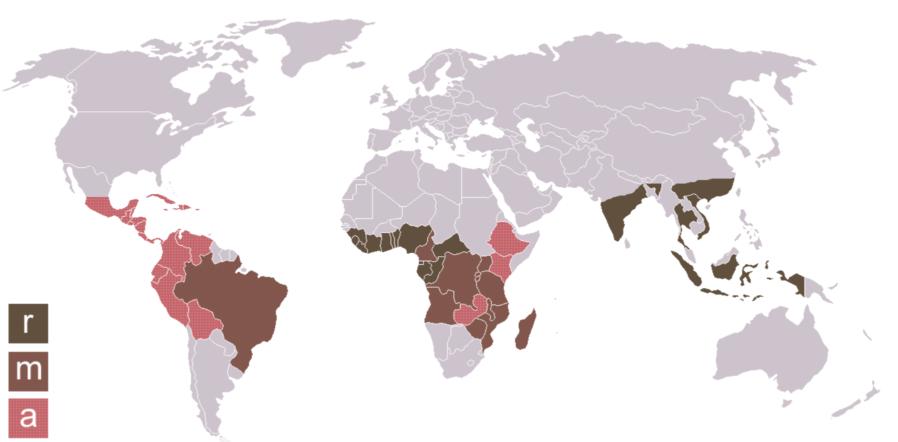
Espresso is 8 – 10 % w/w

Coffee is kind of a big deal to other countries, too:

Burundi — 25% GDP (~$8B) is coffee, 90% population employed

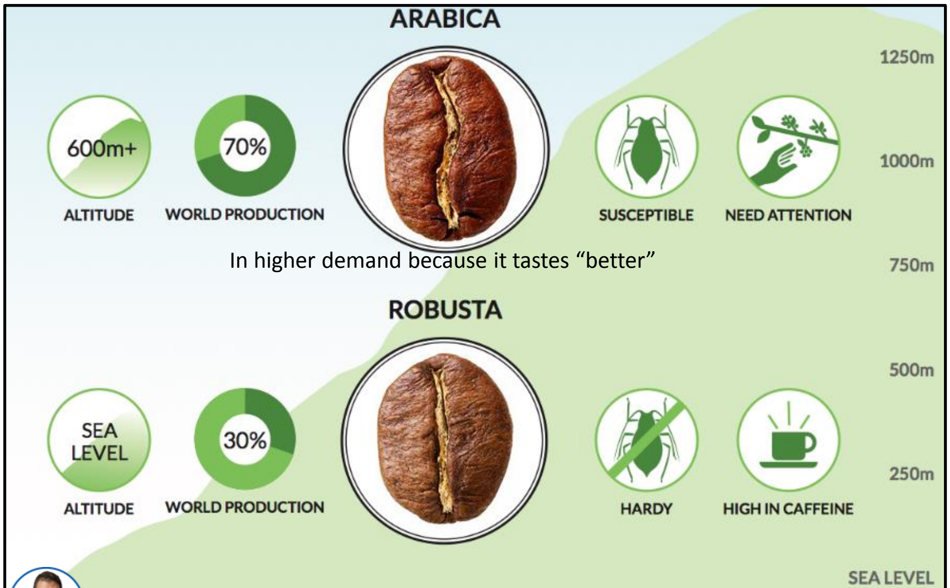
The Bean Belt

The balance between low CO_2 concentrations and high temperature



Microclimates are extremely important, and very poorly studied.

PLoS ONE, **2012**, *7*, e47981

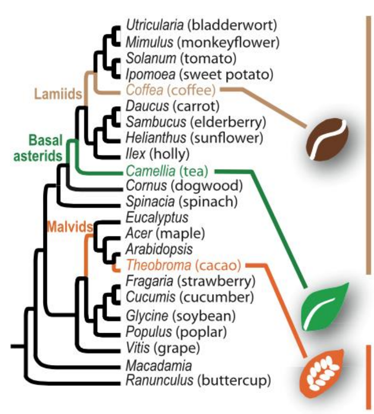


We have the genome for both Robusta and Arabica

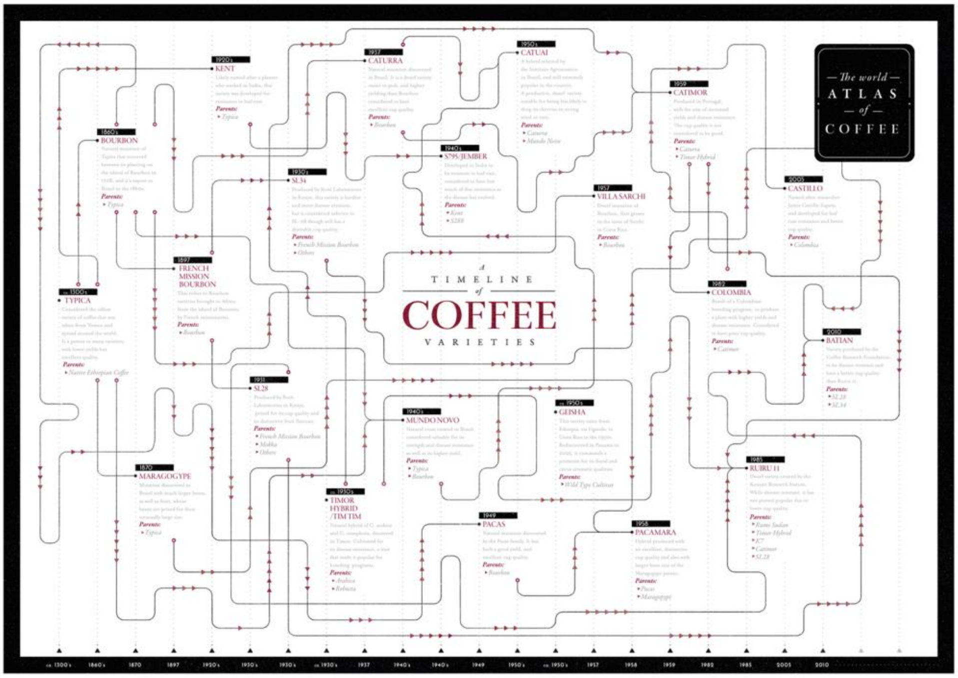
PLANT GENOMICS

The coffee genome provides insight into the convergent evolution of caffeine biosynthesis

France Denoeud,[1,2,3] Lorenzo Carretero-Paulet,[4] Alexis Dereeper,[5] Gaëtan Droc,[6] Romain Guyot,[7] Marco Pietrella,[8] Chunfang Zheng,[9] Adriana Alberti,[1] François Anthony,[5] Giuseppe Aprea,[8] Jean-Marc Aury,[1] Pascal Bento,[1] Maria Bernard,[1] Stéphanie Bocs,[6] Claudine Campa,[7] Alberto Cenci,[5,10] Marie-Christine Combes,[5] Dominique Crouzillat,[11] Corinne Da Silva,[1] Loretta Daddiego,[12] Fabien De Bellis,[6] Stéphane Dussert,[7] Olivier Garsmeur,[6] Thomas Gayraud,[7] Valentin Guignon,[10] Katharina Jahn,[9,13,14] Véronique Jamilloux,[15] Thierry Joët,[7] Karine Labadie,[1] Tianying Lan,[4,16] Julie Leclercq,[6] Maud Lepelley,[11] Thierry Leroy,[6] Lei-Ting Li,[17] Pablo Librado,[18] Loredana Lopez,[12] Adriana Muñoz,[19,20] Benjamin Noel,[1] Alberto Pallavicini,[21] Gaetano Perrotta,[12] Valérie Poncet,[7] David Pot,[6] Priyono,[22] Michel Rigoreau,[11] Mathieu Rouard,[10] Julio Rozas,[18] Christine Tranchant-Dubreuil,[7] Robert VanBuren,[17] Qiong Zhang,[17] Alan C. Andrade,[23] Xavier Argout,[6] Benoît Bertrand,[24] Alexandre de Kochko,[7] Giorgio Graziosi,[21,25] Robert J Henry,[26] Jayarama,[27] Ray Ming,[17] Chifumi Nagai,[28] Steve Rounsley,[29] David Sankoff,[9] Giovanni Giuliano,[8] Victor A. Albert,[4*] Patrick Wincker,[1,2,3*] Philippe Lashermes[5*]



Science, **2014**, *345*, 1181



Coffee begins life as a fruit

Inevitably the fruit is removed to yield a green seed (~11% moisture content)

Fruit or mucilage Parchment Seed

Processing methods

The stage in which coffee is dried

Natural process **Pulped** **Washed process**

Fruit or mucilage Parchment Seed

The chemistry of each processing method is widely unknown

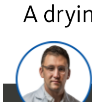
All coffee is then fermented for ~24 hours

Naturals historically came from places with water scarcity or environment in mind

Yemen, parts of Ethiopia, and more recently Brazil

A drying facility in Ethiopia

Defective naturals are UV active
Why?



Int. J. Food Prop., **2017**, 20, S331

The ‘*best*’ coffees in the world

Kopi Luwak (Civet) — fallacy

The ‘*best*’ coffees in the world

fact

No particular country dependence

Although Brazilian, Sumatran, Vietnamese and Hawaii are typically the lowest scoring

Panama Geishas are typically the award winners

Natural and Washed

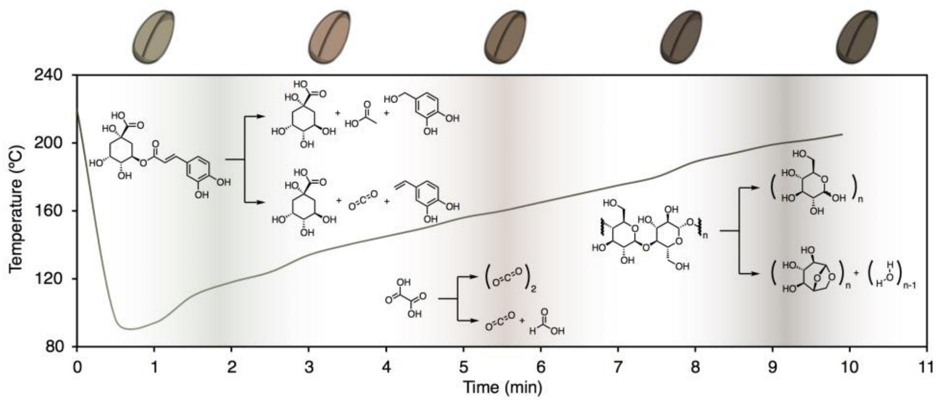
Hendon Materials Simulation

Roasting

Hendon Materials Simulation

The roast profile

Kinetics: Gradient and time determine flavor development



Sci. Rep., 2016, *6*, 24483

45

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Dark roast coffee contains more caffeine?

Fallacy

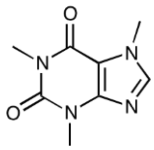


Table II. Caffeine Content of Espresso and Brewed Specialty Coffees

Coffee and Origin	Amount	Caffeine Dose (mg)
Espresso coffees		
Big Bean Espresso, 1-shot	1 shot	75.8
Big Bean Espresso, 2 short shots	2 short shots	140.4
Big Bean Espresso, 2 tall shots	2 tall shots	165.3
Starbucks Espresso, regular, small	1 shot	58.1
Hampden Café Espresso	2 shots	133.5
Einstein Bros® Espresso, double	2 shots	185.0
Brewed specialty coffees		
Big Bean, regular	16 oz	164.7
Big Bean Boat Builders Blend, regular	16 oz	147.6
Big Bean Organic Peru Andes Gold, regular, country origin, Peru	16 oz	186.0
Big Bean French Roast, regular	16 oz	179.8
Big Bean Ethiopian Harrar, regular, country origin, Ethiopia	16 oz	157.1
Big Bean Italian Roast, regular, country origin, Brazil	16 oz	171.8
Big Bean Costa Rican French Roast, regular, country origin, Costa Rica	16 oz	245.1
Big Bean Kenya AA, regular, country origin, Kenya	16 oz	204.9
Big Bean Sumatra Mandheling, regular, country origin, Indonesia	16 oz	168.5
Hampden Café Guatemala Antigua	16 oz	172.7
Starbucks regular	16 oz	259.3
Royal Farms regular	16 oz	225.7
Dunkin' Donuts regular	16 oz	143.4
Einstein Bros regular	16 oz	206.3

J. Anal. Toxic., **2003**, *27*, 520

Some chemistry in roasted coffee

Table I. Coffee Volatiles Identified in the Present Investigation[a]

Compound	References
Hydrocarbons	
Isoprene	Rhoades, 1958, 1960
Alcohols	
Methanol	Reichstein and Staudinger, 1962b
Ethanol	Rhoades, 1958, 1960
2-Propanol	
3-Methylbut-2-en-1-ol	Stoll *et al.*, 1967
Linalool	Stoll *et al.*, 1967
cis-Linalool oxide	Stoll *et al.*, 1967
trans-Linalool oxide	
Aldehydes	
Ethanal	Reichstein and Staudinger, 1926b
Propanal	Zlatkis and Sivetz, 1960
2-Methylpropanal	Rhoades, 1958, 1960
n-Butanal	Rhoades, 1958, 1960
3-Methylbutanal	Rhoades, 1958, 1960
2-Methylbutanal	Reichstein and Staudinger, 1926b
n-Pentanal	Zlatkis and Sivetz, 1960
2-Methylbut-2-en-1-al	Sullivan *et al.*, 1959
m-Tolualdehyde (tentative)	
Ketones	
Propanone	Bernheimer, 1880
Butanone	Rhoades, 1958, 1960
3-Hexanone	Stoll *et al.*, 1967
trans-2-Penten-4-one	
Cyclopentanone	Gianturco *et al.*, 1966
Hexane-2,5-dione	
Heptane-2,5-dione	

Compound	References
Lactones	
γ-Butyrolactone	Viani *et al.*, 1965
γ-Valerolactone	
α-Methyl-γ-butyrolactone	
2,3-Dimethylbut-2-en-1,4-olide	
3,4-Dimethylbut-2-en-1,4-olide	
2,3,4-Trimethylbut-2-en-1,4-olide	
Esters	
Methyl formate	Rhoades, 1958, 1960
Methyl acetate	Sullivan *et al.*, 1959
Methyl propionate	Merritt *et al.*, 1966
Methyl salicylate	Stoll *et al.*, 1967
Methyl phenylacetate	
Ethyl formate	Zlatkis and Sivetz, 1960
Ethyl acetate	Gianturco *et al.*, 1966
Isopropyl formate	
Isoamyl acetate	
β-Phenylethyl formate	Stoll *et al.*, 1967
Phenols and Phenol Ethers	
Phenol	Reichstein and Staudinger, 1926b
o-Cresol	Stoll *et al.*, 1967
2,6-Dimethylphenol	Stoll *et al.*, 1967
Guaiacol	Reichstein and Staudinger, 1926b
4-Ethylguaiacol	Gianturco *et al.*, 1966
4-Vinylguaiacol	Reichstein and Staudinger, 1926b
o-Hydroxyacetophenone	Stoll *et al.*, 1967
Sulfur-containing	

Nature, **1966**, *210*, 1358

J. Food Sci., **2016**, *81*, S2997

Hendon Materials Simulation

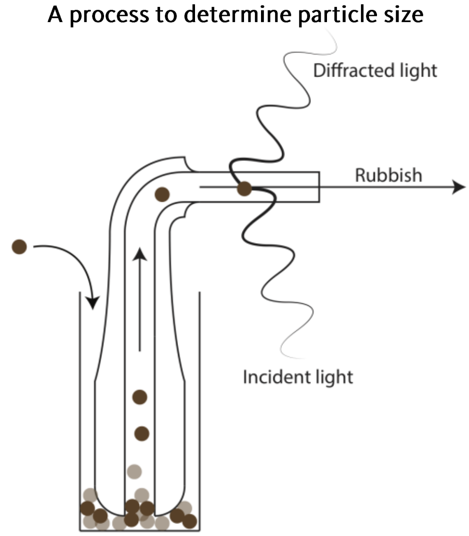
Grinding

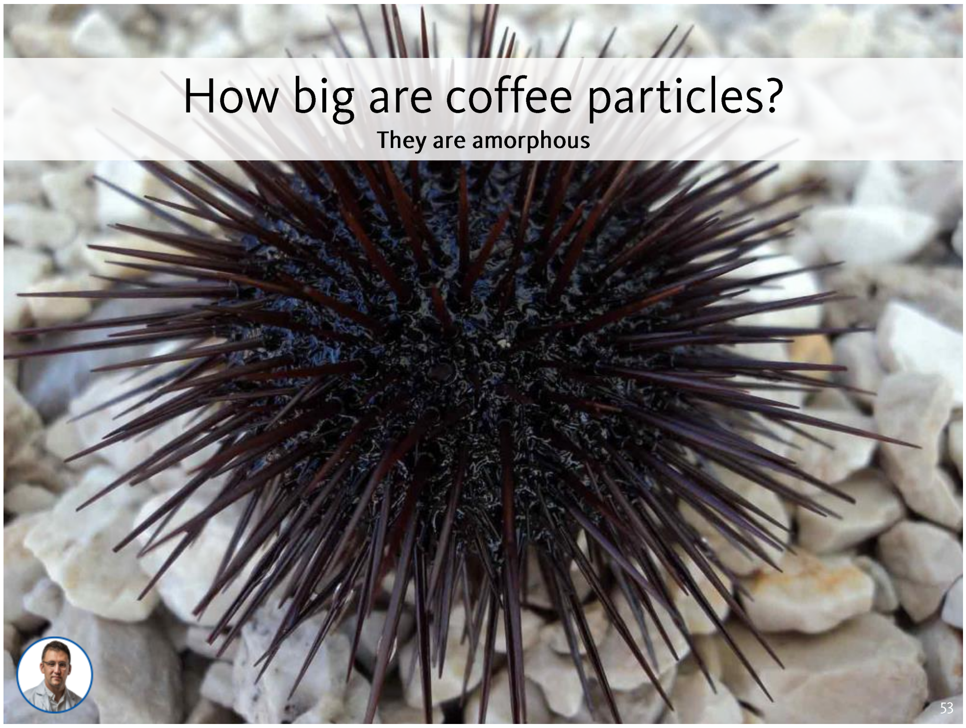
Conical vs. flat burrs

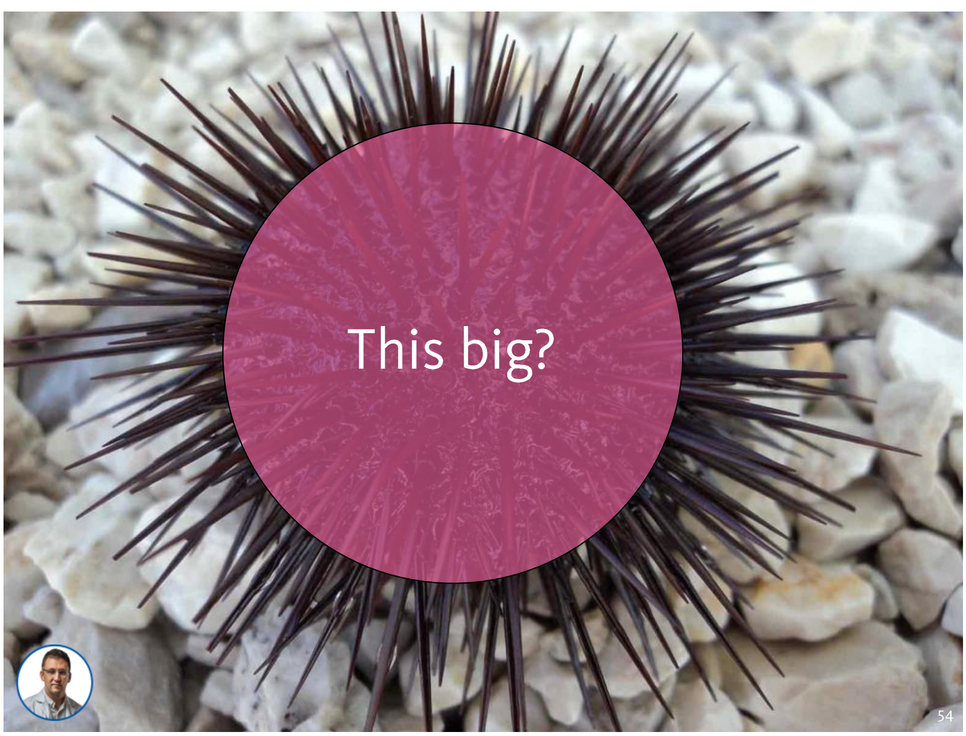
Different burrs produce different particle size distributions

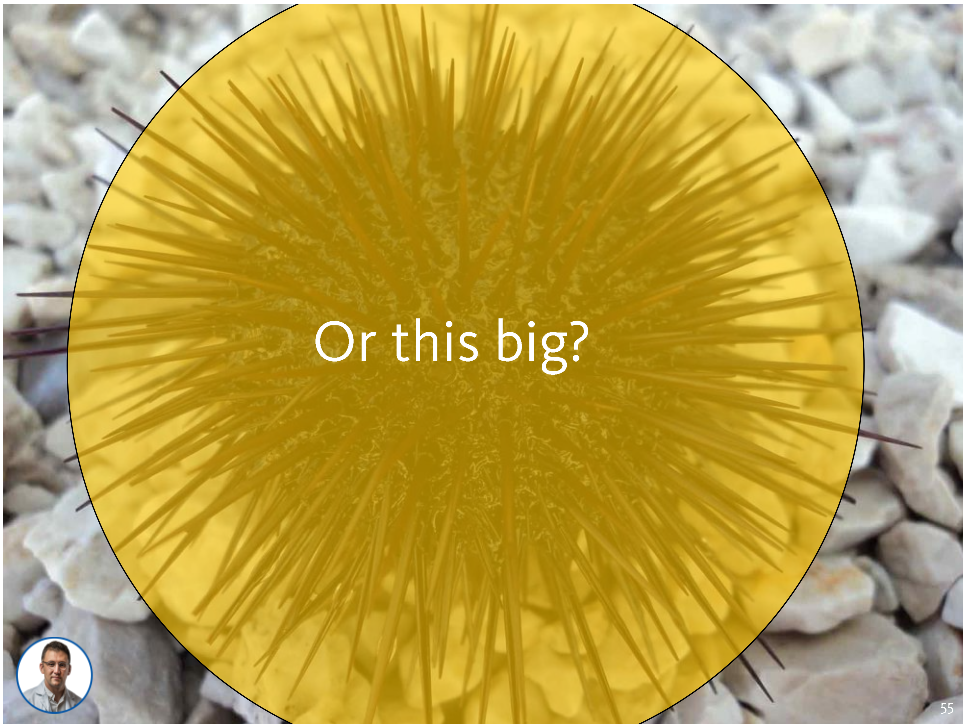
Laser diffraction particle size analysis

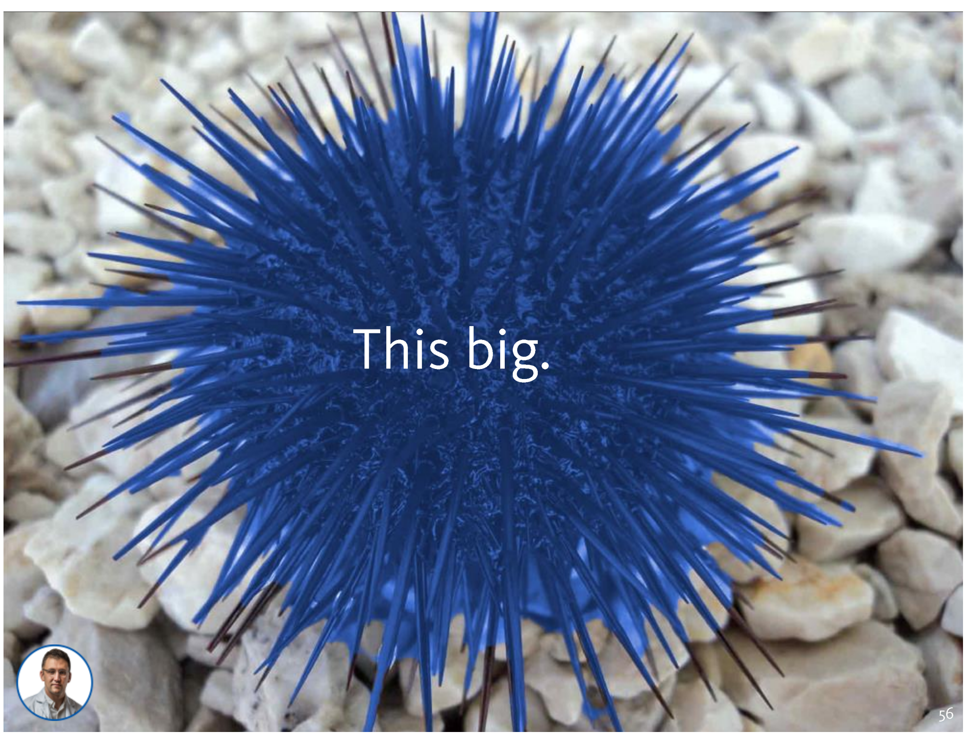
A process to determine particle size



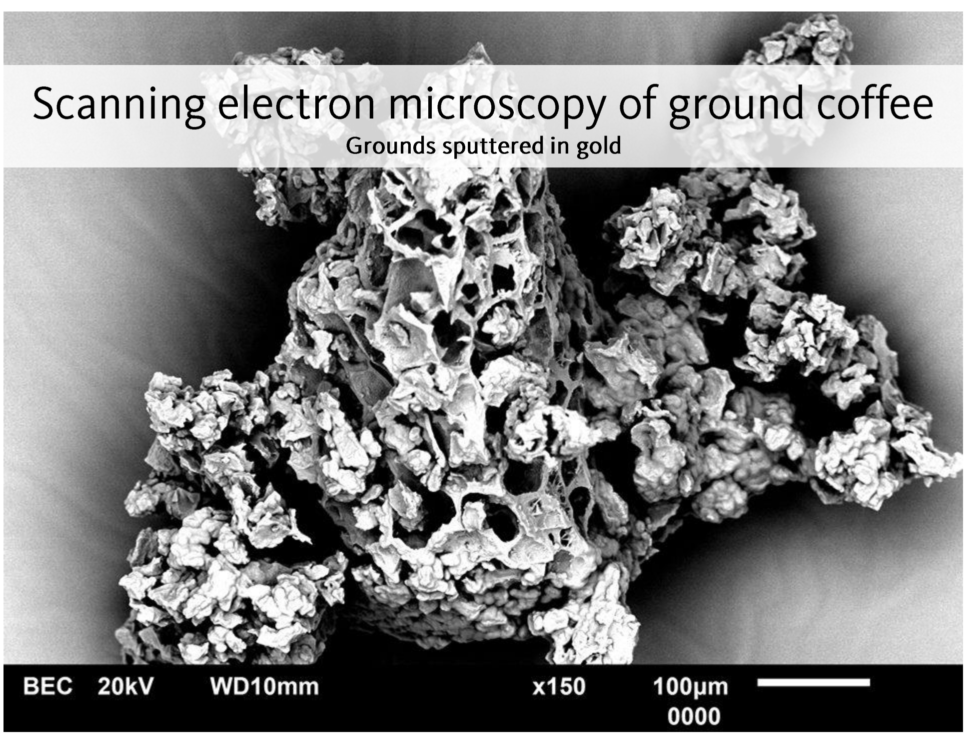

How big are coffee particles?
They are amorphous
53


This big?
54


Or this big?
55

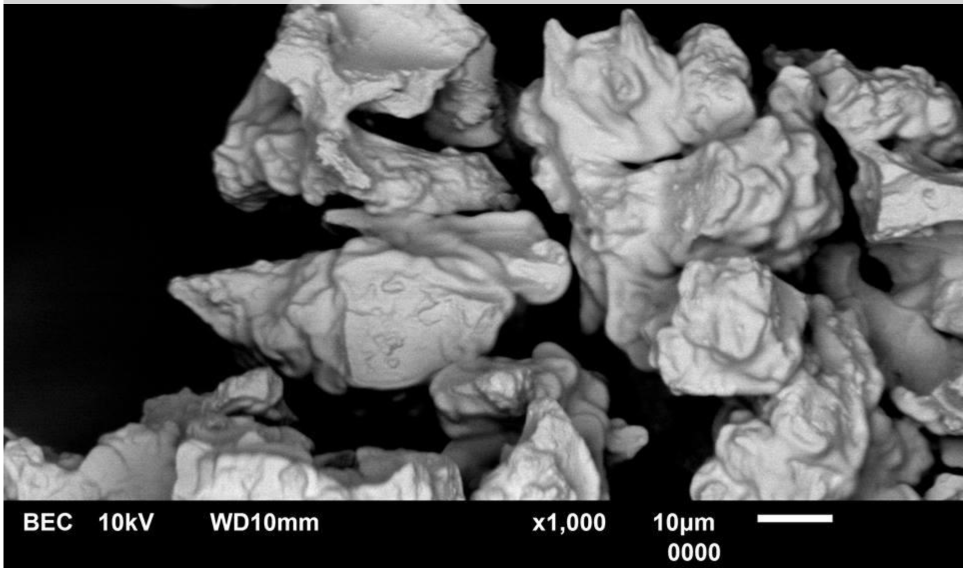

This big.
56


We measure this
conservative surface area to volume
57


Scanning electron microscopy of ground coffee
Grounds sputtered in gold
BEC 20kV WD10mm x150 100µm
0000

They don’t appear to be very spherical

Grounds sputtered in gold



Journal of Food Engineering 150 (2015) 106–116

Contents lists available at ScienceDirect

Journal of Food Engineering

journal homepage: www.elsevier.com/locate/jfoodeng

A new methodology to estimate the steady-state permeability of roast and ground coffee in packed beds

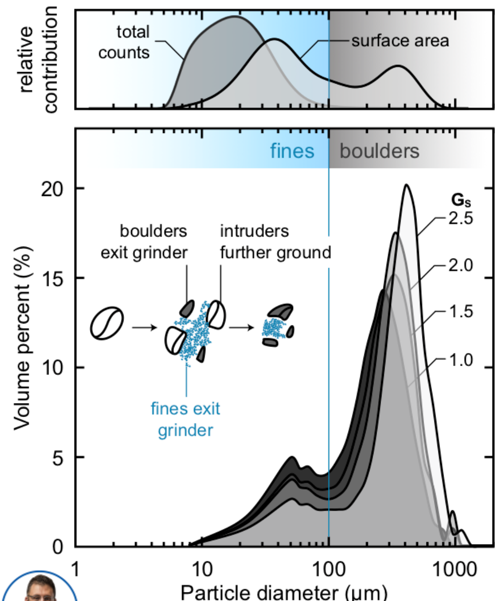
B.R. Corrochano [a,b,*], J.R. Melrose [b], A.C. Bentley [b], P.J. Fryer [a], S. Bakalis [a]

[a] Centre for Formulation Engineering, Department of Chemical Engineering, University of Birmingham, Edgbaston, Birmingham B15 2TT, UK
[b] Mondelēz International, Coffee Global Centre of Excellence, Ruscote Avenue, Banbury OX16 2QU, UK

- Little particles are closely approximated by a sphere
- Coffee **is** a bit porous (BET measurements are ongoing)
- **Spherical approximation is good enough**

J. Food Eng., **2015**, *150*, 106

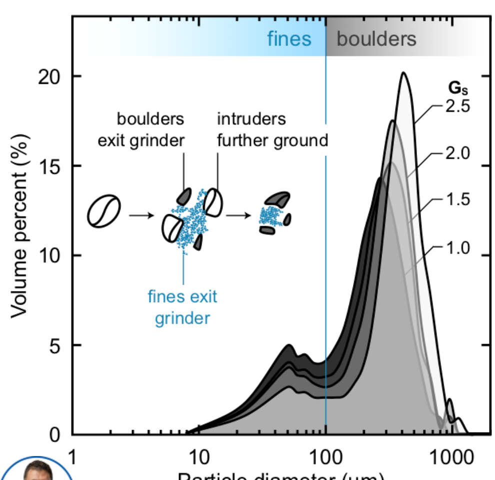
60



The effect of changing grind setting

Grinding finer make more fine particulates, and small large particulates

Fracturing of coffee likely proceeds through volcanic rock decomposition pathway



A theoretical explanation of grain size distributions in explosive rock fragmentation

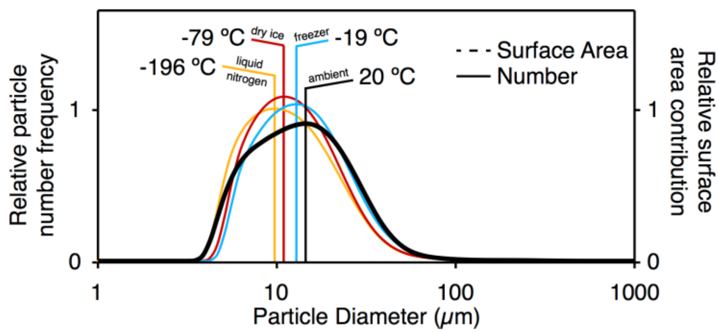
A. C. Fowler[1,2] and Bettina Scheu[3]

[1]MACSI, University of Limerick, Limerick, Republic of Ireland
[2]OCIAM, University of Oxford, Oxford, UK
[3]Earth and Environmental Sciences, LMU München, München, Germany

ACF, 0000-0002-2062-6372

Hendon Materials Simulation

Cooling coffee before grinding augments the fine particle sizes



Sci. Rep., 2016, 6, 24483

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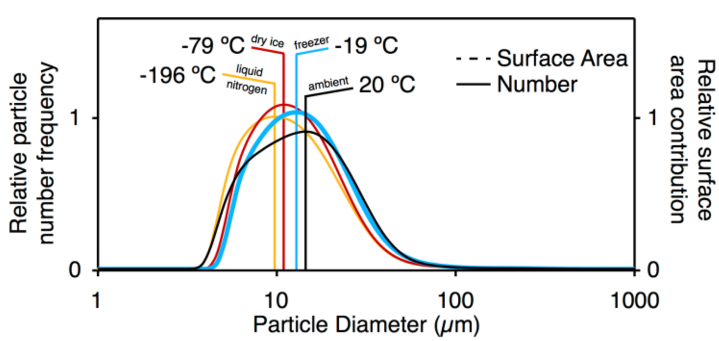
Hendon Materials Simulation

Cooling coffee before grinding augments the fine particle sizes



Sci. Rep., 2016, 6, 24483

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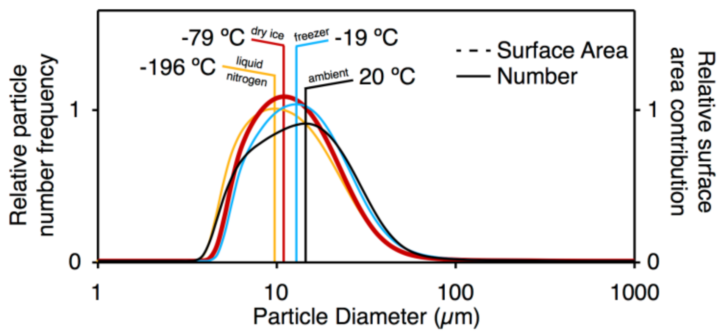
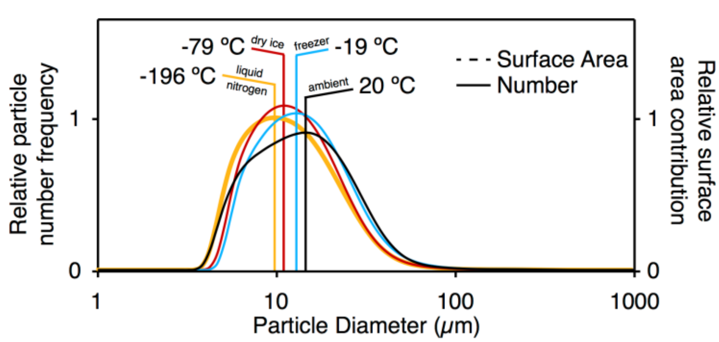
Cooling coffee before grinding augments the fine particle sizes

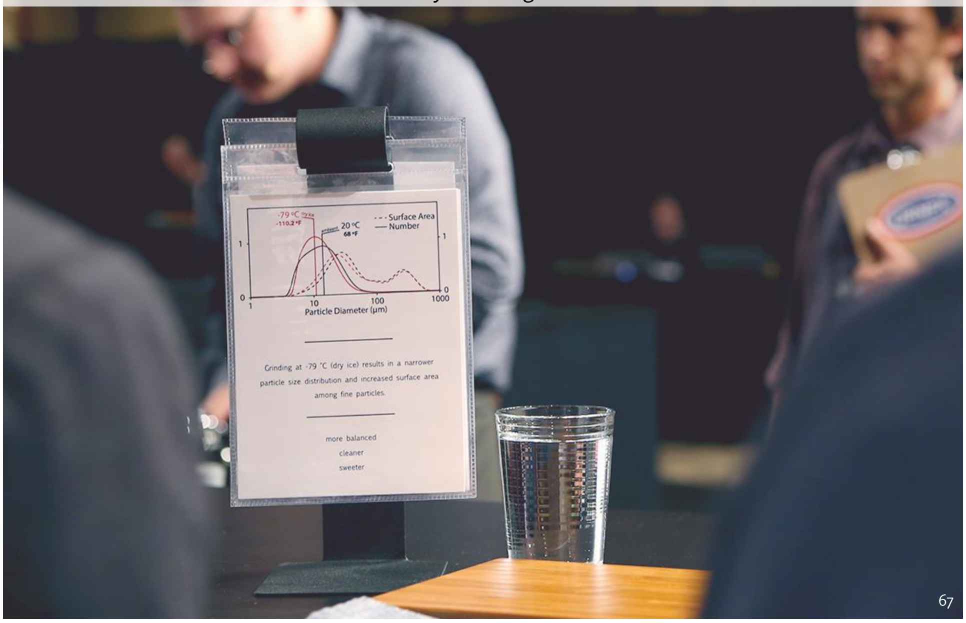


Cooling coffee before grinding augments the fine particle sizes



Hendon Materials Simulation

USA Barista Champion 2017
Kyle Ramage



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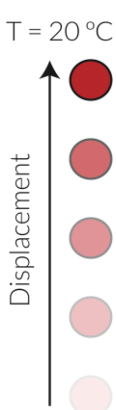
Hendon Materials Simulation

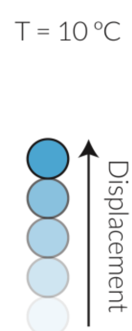
Added benefits from cooled coffee

preservation



from to the Arrhenius equation
(and later formalized by Eyring)

'...the rate of a reaction doubles
for every 10 °C increase in T...'



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Hendon Materials Simulation

If you are going to store coffee in the fridge or freezer, store it

air tight

roasted coffee is extremely hygroscopic

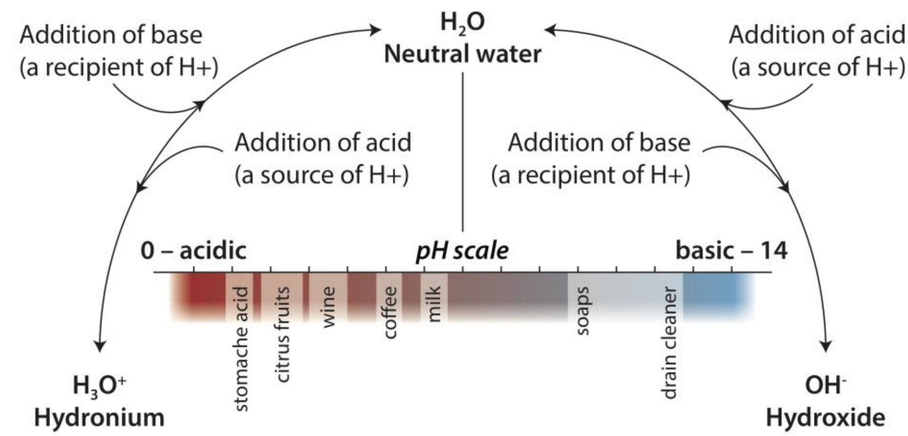
Image courtesy of Michael Cameron

Water chemistry

72

The water molecule

water is both an acid and a base



Sci. Rep., **2018**, *8*, 16030

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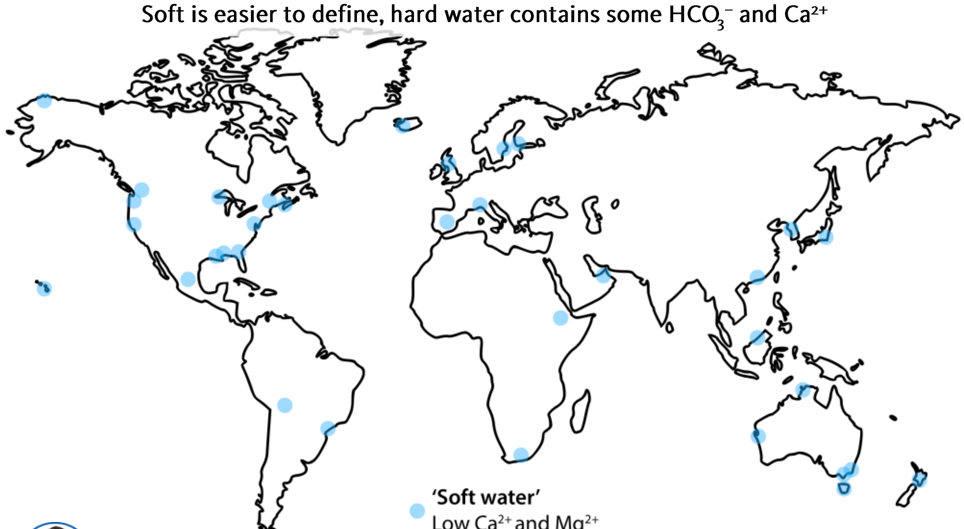
Geographical dependence on water chemistry

Soft is easier to define, hard water contains some HCO_3^- and Ca^{2+}



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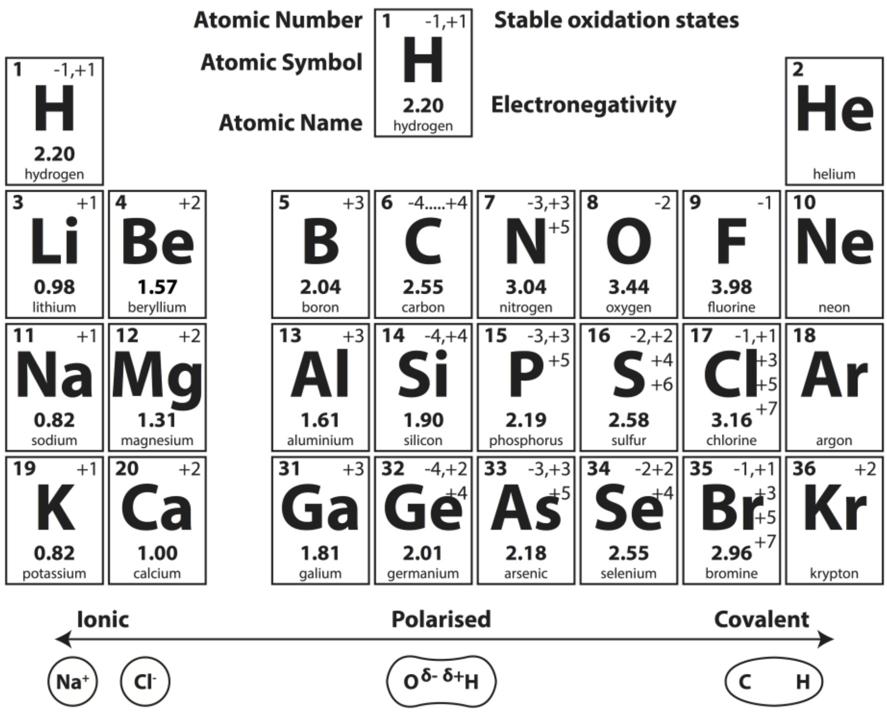
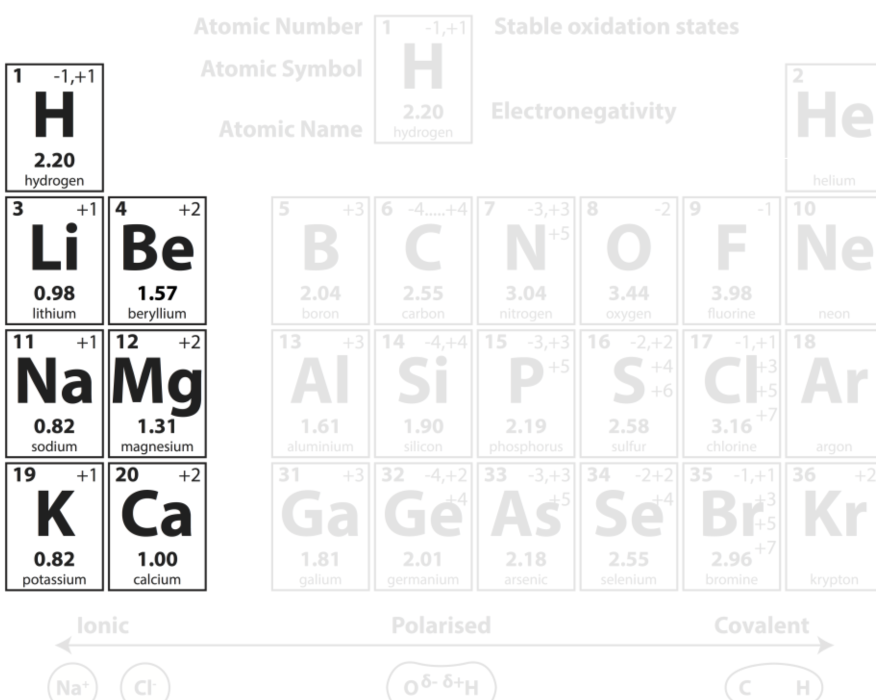
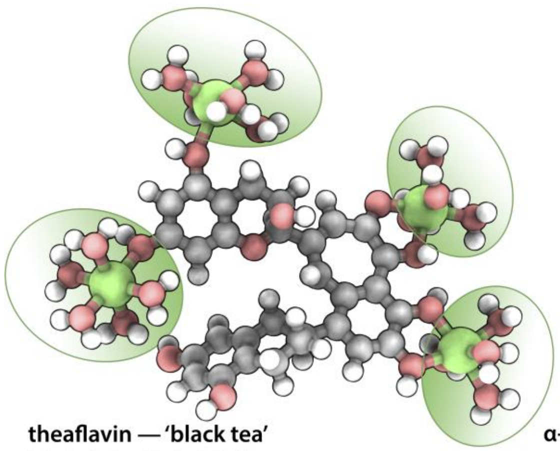

Atomic Number
Atomic Symbol
Atomic Name
Stable oxidation states
Electronegativity
1 -1,+1 H 2.20 hydrogen
2 He helium
3 +1 Li 0.98 lithium
4 +2 Be 1.57 beryllium
5 +3 B 2.04 boron
6 -4.....+4 C 2.55 carbon
7 -3,+3 +5 N 3.04 nitrogen
8 -2 O 3.44 oxygen
9 -1 F 3.98 fluorine
10 Ne neon
11 +1 Na 0.82 sodium
12 +2 Mg 1.31 magnesium
13 +3 Al 1.61 aluminium
14 -4,+4 Si 1.90 silicon
15 -3,+3 +5 P 2.19 phosphorus
16 -2,+2 +4 +6 S 2.58 sulfur
17 -1,+1 +3 +5 +7 Cl 3.16 chlorine
18 Ar argon
19 +1 K 0.82 potassium
20 +2 Ca 1.00 calcium
31 +3 Ga 1.81 galium
32 -4,+2 +4 Ge 2.01 germanium
33 -3,+3 +5 As 2.18 arsenic
34 -2+2 +4 Se 2.55 selenium
35 -1,+1 +3 +5 +7 Br 2.96 bromine
36 +2 Kr krypton
Ionic
Polarised
Covalent
Na+
Cl-
O δ- δ+ H
C H


1 -1,+1 H 2.20 hydrogen
3 +1 Li 0.98 lithium
4 +2 Be 1.57 beryllium
11 +1 Na 0.82 sodium
12 +2 Mg 1.31 magnesium
19 +1 K 0.82 potassium
20 +2 Ca 1.00 calcium

Metals binding to polar molecules

A high fidelity perspective of ionic strength



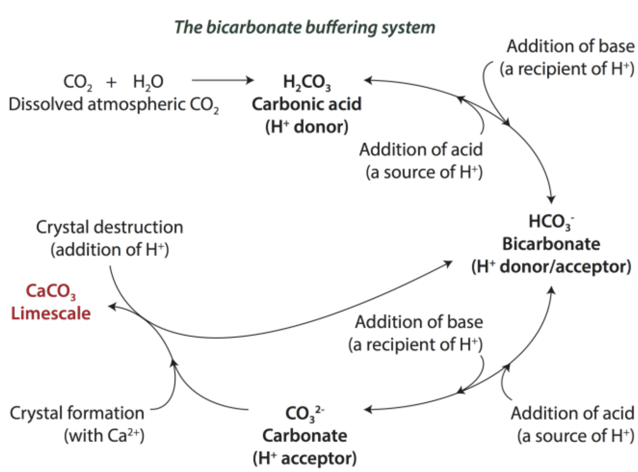
theaflavin — 'black tea'
binds to hydrated Ca^{2+}
through oxygen

α-pinene — 'chamomile'
does not bind to Ca^{2+}
α-pinene is non-polar

J. Agric. Food Chem., **2014**, *62*, 4947

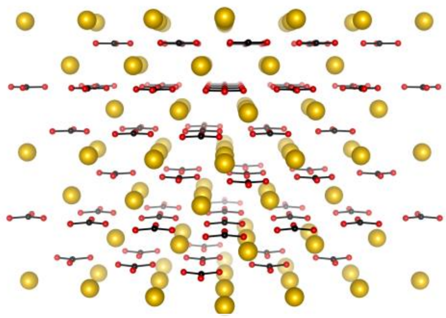
Bicarbonate (HCO_3^-)

The buffer – minimizing pH fluctuations



Calcium carbonate

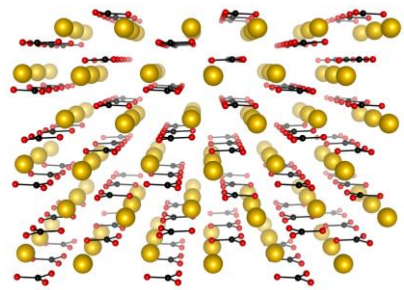
$Ca^{2+} + 2(HCO_3^-)$ to yield $CaCO_3$, a white insoluble solid



Calcite

Sheet-like

Shows up on the bottom of flat kettles



Aragonite

Jagged

Found on the end of taps

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Audience Challenge Question

ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT

Is your tap water high in Ca^{2+}, HCO_3^-, and other minerals?

In other words, is your water hard?

- My water is hard
- My water is soft
- I don’t have a clue

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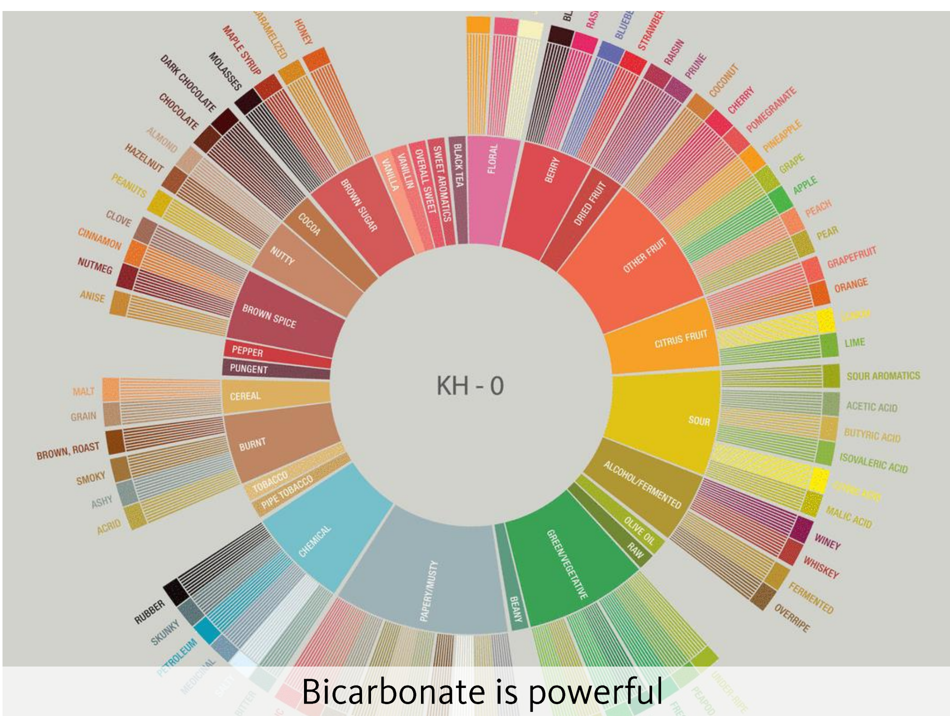
FLORAL
FRUITY
SOUR/FERMENTED
GREEN/VEGETATIVE
OTHER
ROASTED
SPICES
NUTTY/COCOA
SWEET
BLACK TEA
BERRY
DRIED FRUIT
OTHER FRUIT
CITRUS FRUIT
SOUR
ALCOHOL/FERMENTED
OLIVE OIL
RAW
BEANY
PAPERY/MUSTY
CHEMICAL
PIPE TOBACCO
TOBACCO
BURNT
CEREAL
PUNGENT
PEPPER
BROWN SPICE
NUTTY
COCOA
BROWN SUGAR
VANILLA
VANILLIN
OVERALL SWEET
SWEET AROMATICS
HONEY
MAPLE SYRUP
MOLASSES
DARK CHOCOLATE
CHOCOLATE
ALMOND
HAZELNUT
PEANUTS
CLOVE
CINNAMON
NUTMEG
ANISE
MALT
GRAIN
BROWN, ROAST
SMOKY
ASHY
ACRID
RUBBER
SKUNKY
PETROLEUM
MEDICINAL
SALTY
BITTER
UNDER-RIPE
PEAPOD
FRESH
RAISIN
PRUNE
COCONUT
CHERRY
POMEGRANATE
PINEAPPLE
GRAPE
APPLE
PEACH
PEAR
GRAPEFRUIT
ORANGE
LIME
SOUR AROMATICS
ACETIC ACID
BUTYRIC ACID
ISOVALERIC ACID
MALIC ACID
WINEY
WHISKEY
FERMENTED
OVERRIPE


KH - 0
Bicarbonate is powerful
FLORAL
BLACK TEA
BERRY
DRIED FRUIT
OTHER FRUIT
CITRUS FRUIT
SOUR
ALCOHOL/FERMENTED
OLIVE OIL
RAW
GREEN/VEGETATIVE
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SMOKY
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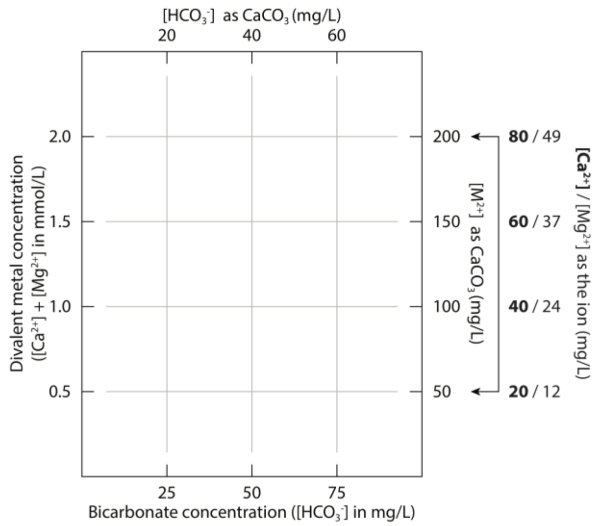
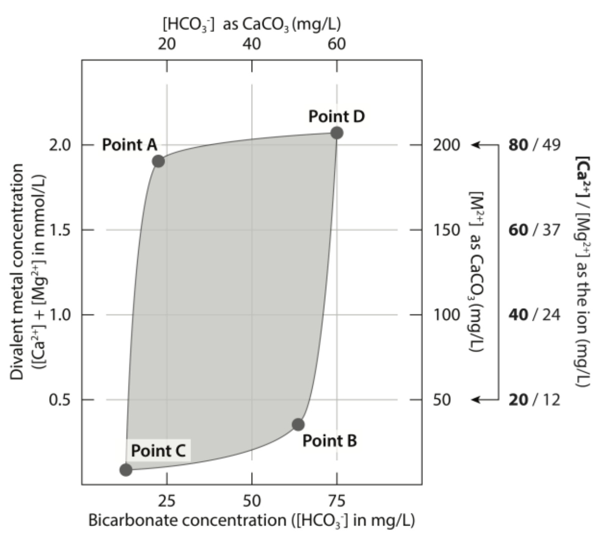
SKUNKY
PETROLEUM
RAISIN
PRUNE
COCONUT
CHERRY
POMEGRANATE
PINEAPPLE
GRAPE
APPLE
PEACH
PEAR
GRAPEFRUIT
ORANGE
LIME
SOUR AROMATICS
ACETIC ACID
BUTYRIC ACID
ISOVALERIC ACID
MALIC ACID
WINEY
WHISKEY
FERMENTED
OVERRIPE

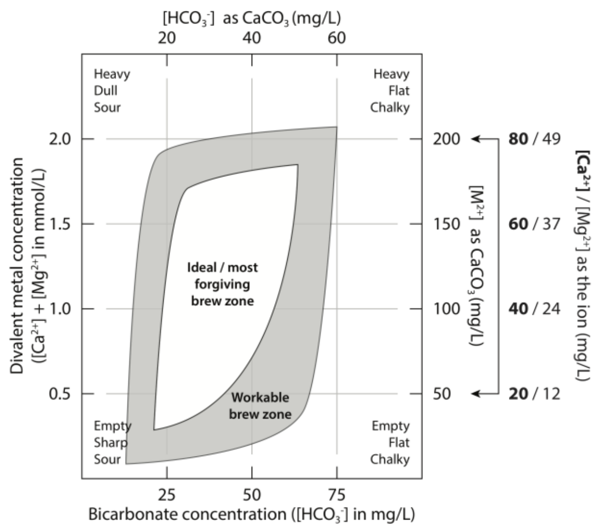
What water do we want for coffee?



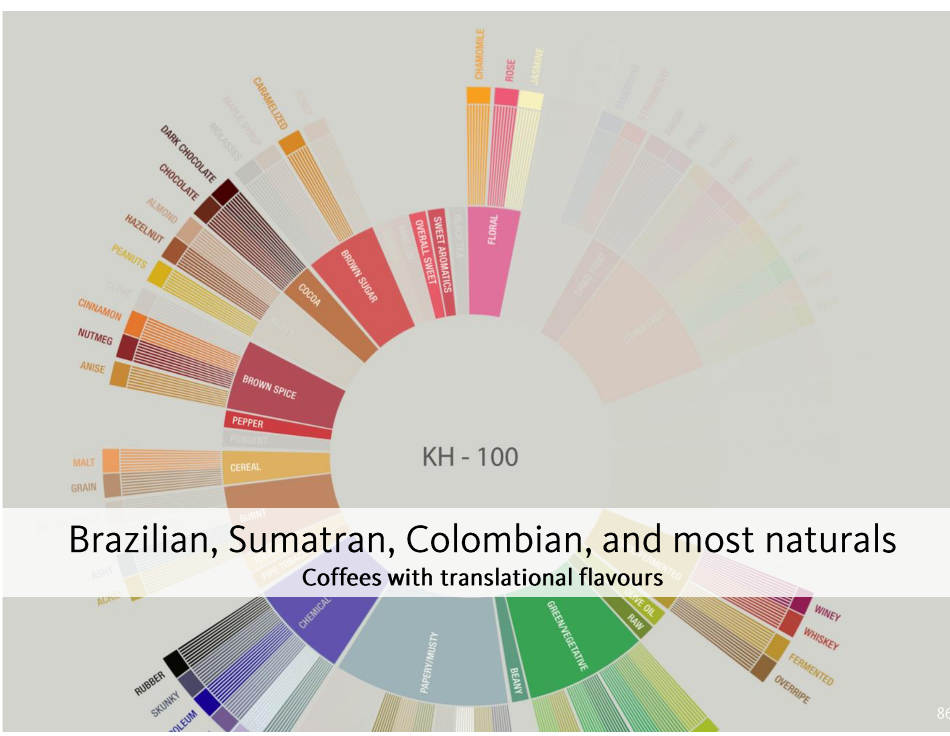
Not too much of anything



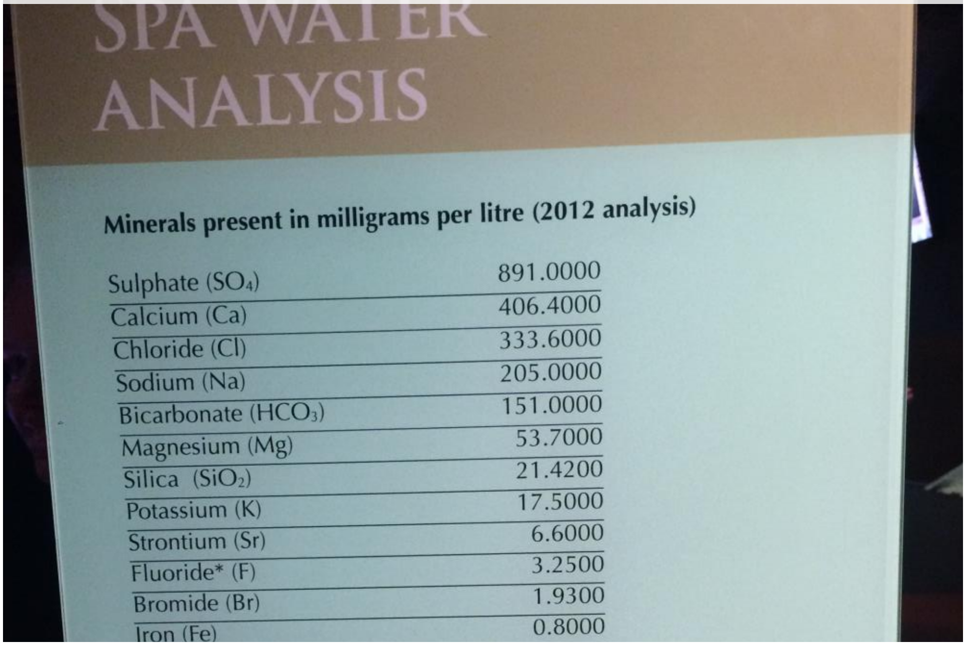
Our empirical ideal brew zone



Water For Coffee 2, 2019



The Roman Baths were Really Hard



SPA WATER ANALYSIS

Minerals present in milligrams per litre (2012 analysis)

Sulphate (SO_4)	891.0000
Calcium (Ca)	406.4000
Chloride (Cl)	333.6000
Sodium (Na)	205.0000
Bicarbonate (HCO_3)	151.0000
Magnesium (Mg)	53.7000
Silica (SiO_2)	21.4200
Potassium (K)	17.5000
Strontium (Sr)	6.6000
Fluoride* (F)	3.2500
Bromide (Br)	1.9300
Iron (Fe)	0.8000

Hendon Materials Simulation

Some handy water recipes

for better or worse

The front and center

0.25 g/L $MgSO_4.7H_2O$ (epsom salt)

~25 ppm Mg^{2+} as Mg^{2+}

0.05 g/L $NaHCO_3$ (baking soda)

~35 ppm HCO_3^- as HCO_3^-

The 7 n' 7

0.3 g/L $CaSO_4.2H_2O$ (gypsum salt)

~70 ppm Ca^{2+} as Ca^{2+}

0.11 g/L $NaHCO_3$ (baking soda)

~70 ppm HCO_3^- as HCO_3^-

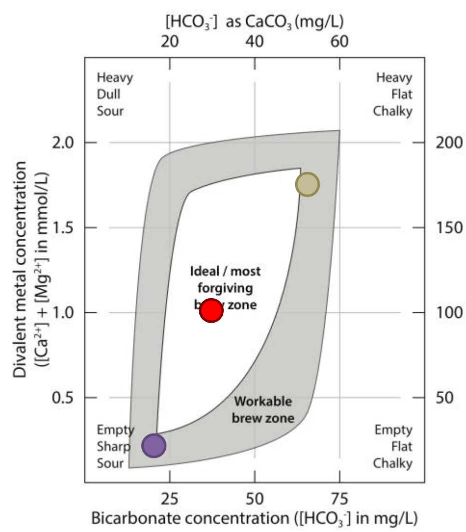
The double rizzi banger

0.05 g/L $MgSO_4.7H_2O$ (gypsum salt)

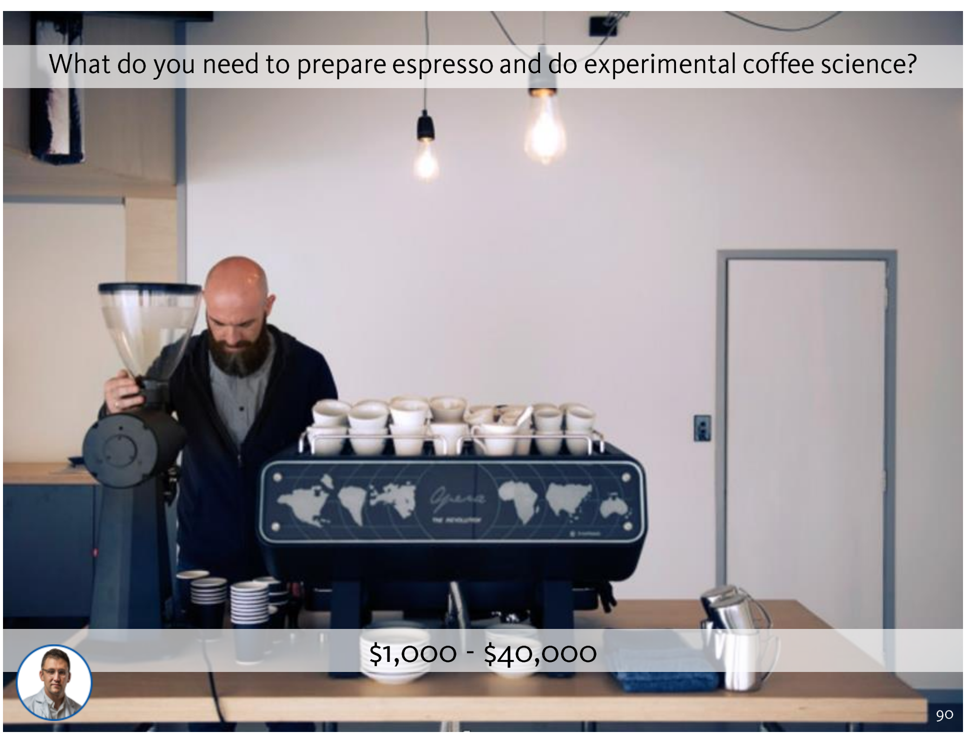
~5 ppm Mg^{2+} as Mg^{2+}

0.02 g/L $NaHCO_3$ (baking soda)

~15 ppm HCO_3^- as HCO_3^-



Brewing


What do you need to prepare espresso and do experimental coffee science?
$1,000 - $40,000

Hendon Materials Simulation

The definition of ***espresso***

The Specialty Coffee Association (SCA) defines espresso as “a **25-35mL** beverage prepared from **7-9 grams of coffee** through which clean water of 195°- 205 °F (**92°-95°C**) has been forced at **9-10 atmospheres of pressure**, and where the grind of the coffee is such that the brewing ‘flow’ time is approximately **20-30 seconds.**”

Hendon Materials Simulation

The definition of ***espresso***

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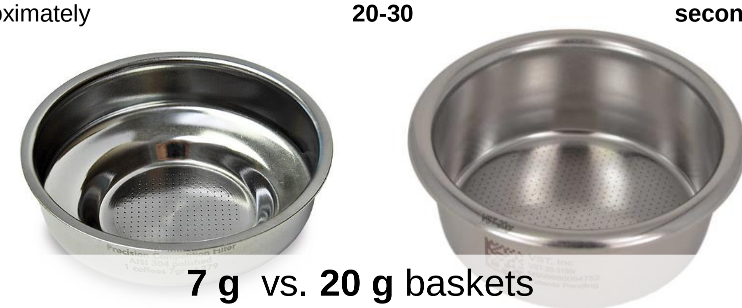


7 g vs. **20 g** baskets

The definition of ***espresso***

The Specialty Coffee Association (SCA) defines espresso as "a **25-35mL** beverage prepared from **7-9 grams of coffee** through which clean water of 195°- 205 °F (**92°-95°C**) has been forced at **9-10 atmospheres of pressure**, and where the grind of the coffee is such that the brewing 'flow' time is approximately **20-30 seconds.**"

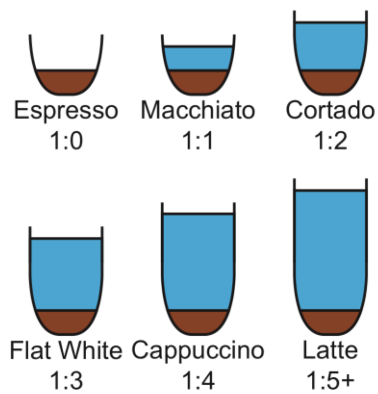
Nobody makes espresso anymore

Time: The one gospel

The Specialty Coffee Association (SCA) defines espresso as "a **25-35mL** beverage prepared from **7-9 grams of coffee** through which clean water of 195°- 205 °F (**92°-95°C**) has been forced at **9-10 atmospheres of pressure**, and where the grind of the coffee is such that the brewing 'flow' time is approximately

20-30 seconds."

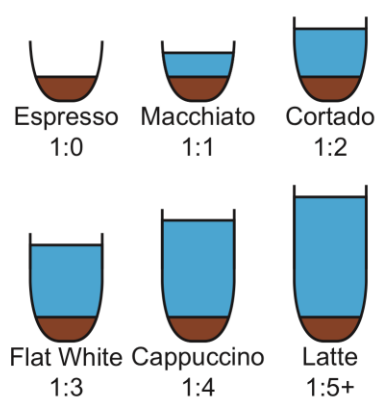
The modern espresso menu



Espresso is a drink prepared with an espresso machine, and typically features about **10% coffee mass per mass of liquid**

Implication: The volume/mass of the espresso determines the volume/mass of milk required to achieve drink definition.

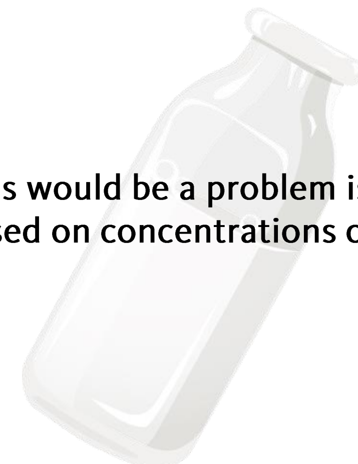
The Australian's ruined everything



A single espresso is half of the volume and physical shot produced when a 20 g basket is used.

A double espresso is the entire liquid produced in a single extraction.

Hendon Materials Simulation



None of this would be a problem is we all made beverages based on concentrations of coffee in milk.

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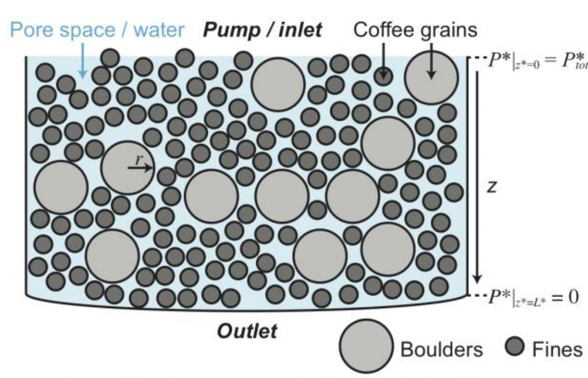
Hendon Materials Simulation

Development of a numerical model for extraction from a granular bed



Ω_s – the volume fraction occupied by coffee grains
Ω_L – the volume fraction occupied by liquid

In preparation

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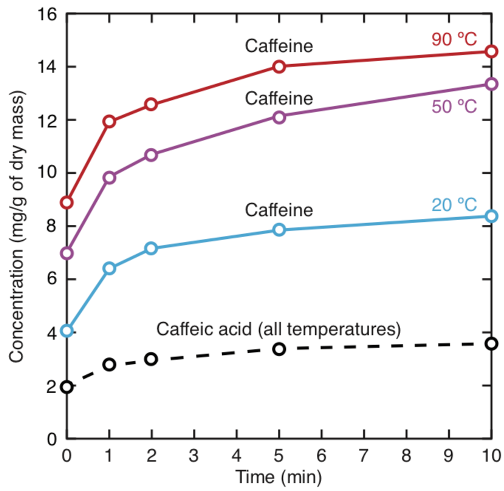
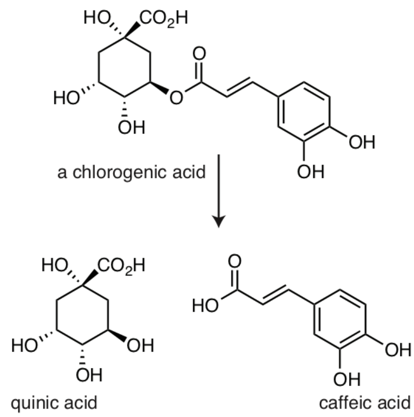
Experimental kinetics

isolating temperature and molecular dissolution rates





Implications, Conclusions, and Future Directions

- Many biochemical unanswered questions in processing (Nature/Pulped/Washed), as well as fermentation stage.
- No quantitative roasting studies on flavor development
- Very few relevant studies on extraction kinetics
- Room for improvement in grinder manufacturing
- Hundreds of other exciting questions, which are the basis for both my coffee lab and also the UC Davis endeavor

The collaborators

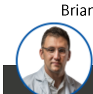
Roasters
George Howell (Boston, MA)
Colonna (Bath, England)
Roseline (Portland, OR)
Tailored (Eugene, OR)
Supreme (Brisbane, Australia)
Spark (Sendai, Japan)
Gracenote (Boston, MA)
Counter Culture (Durham, NC)
Kittel (Montreal, Canada)
Lomi (Paris, France)
Belleville (Paris, France)
Stephen Leighton (Stafford, UK)

Baristas
Maxwell Colonna-Dashwood
Lesley Colonna-Dashwood
Michael Cameron
Dechen Morisco
Brian Sung
Benjamin Put
Charlotte Malaval
Ben Kaminsky
Kyle Ramage
Matt Lewin
Craig Simon
Jérôme Grenier-Desbiens
Hidenori Izaki
Matthew Perger

Equipment manufacturers
Beckman Coulter
Mahlkönig
San Remo
Puqpress
La Marzocco
Reg Barber

Academics
Jamie Foster (Portsmouth, UK)
William Lee (Huddersfield, UK)
Justin Wilkinson (Cambridge, UK)
Zachary C. Kennedy (PNNL, WA)
Sean A. Fontenot (Oregon, OR)
Brent Melot (USC, CA)
Keith, T. Butler (Oxford, UK)
Rory W. Speirs (Melbourne, AUS)

And many many more



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Some actionable information

Brew recipe: **60 g of coffee / L**
The most common mistake in home brewing is using too little coffee and extracting for too long
Coarse grind (French Press, 4 min)
Medium grind (pour over, 2.5 min)
fine grind (Aeropress, 1.25 min)

Water chemistry: **Start with RO/DI/Milli-Q water**
Keep bicarbonate below 50 mg/L
0.25 g/L $MgSO_4.7H_2O$ (epsom salt)
~25 ppm Mg^{2+} as Mg^{2+}
0.05 g/L $NaHCO_3$ (baking soda)
~35 ppm HCO_3^- as HCO_3^-

Coffee preference: *VERY APPROXIMATELY*
Acidic = East Africa, Chocolate and nuts = South/Central America

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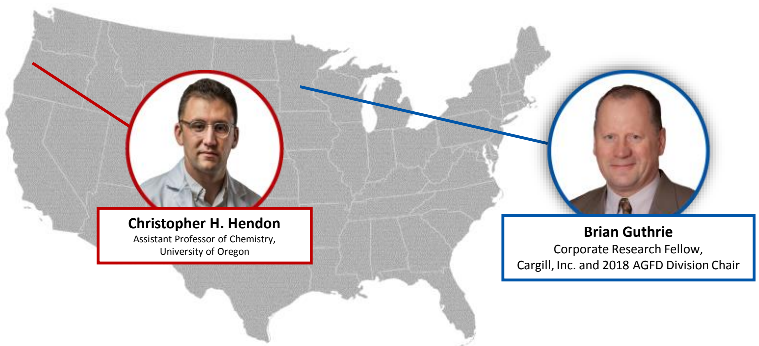

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University of Gothenburg


Alexander Kapustin
AstraZeneca

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ChemRxiv


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ACS Technical Division
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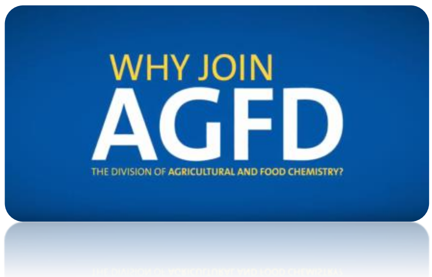

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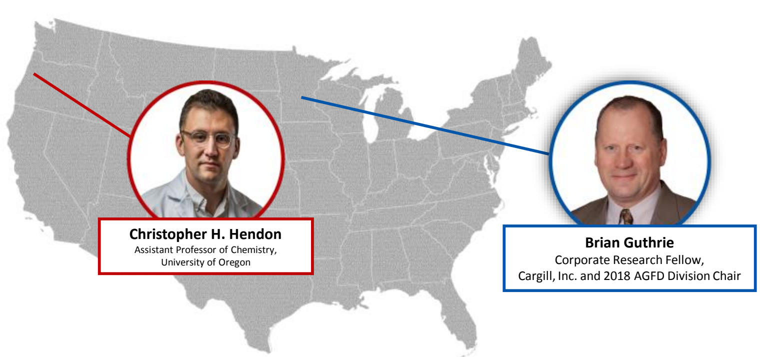
Coffee: *A Chemical and Physical Perspective*



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