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ACS Webinars



Speakers: Jahnavi Phalkey, Science Gallery Bengaluru and Jesse Smith, Science

Moderator: Daryl Boudreaux, Principal, Boudreaux & Associates LLC

Register for Free!

What You Will Learn:

- . The history of water quality analysis and the various scales of water protection that have emerged in the United States over the past 200 years
- . The challenges, limitations, and opportunities of more ontological approaches to the interpretation of water for public audiences
- Why museums and galleries should interpret water not as a singular material that preexists its understanding by scientific or indigenous knowledge, but rather as a multiplicity made by and bound up in systems of bodies, practice, power, and places

Co-produced with: Science History Institute and Chemical & Engineering News



Date: Thursday, January 28, 2021 @ 2-3:30pm ET Speakers: Katrina Knauer, BloCellection Inc. and Philippe Reutenauer, Léa Nature

- . Challenges in recycling of plastics and scaling new depolymerization
- . Chemical pathways for breaking down single-use plastics with an emphasis
- · Synthesis of new polymers from chemically recycled monomers
- the public concerns linked to plastic packaging
- . Mechanical recycling and its limitations and the emerging solutions for

Co-produced with: ACS Division of Polymer Chemistry





Date: Thursday, February 4, 2021 @ 2-3pm ET

Moderator: Glenn Ruskin, American Chemical Society

What You Will Learn:

- . What the world thinks of science during the global pandemic and if
- . What the global public cares about the most as it relates to science
- What specific actions can we all take to advocate for science

Co-produced with: ACS External Affairs & Communications

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ACS Division of Agricultural & Food Chemistry





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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ESPESSO

Chemistry

From First Principles
to Current Challenges

THIS ACS WEBINAR WILL BEGIN SHORTLY...





Espresso Chemistry: From First Principles to Current Challenges





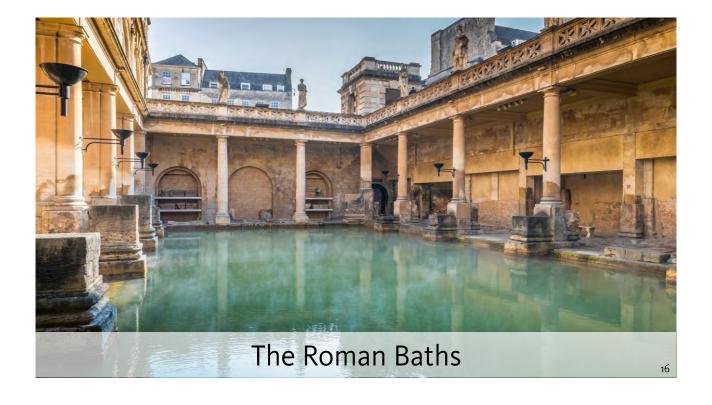
Presentation slides are available now! The edited recording will be made available as soon as possible.

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Hendon Materials Simulation — 2020



Jenna Mancuso
Photoactive MOFs and chemical kinetics



Austin Mroz

Machine learning and
materials theory



Conductive MOFs



Josh Davis
Water dissociation and solid/liquid interfaces



XSEDE

Extreme Science and Engineering Discovery Environment



Jack Yang
Molecular redox and inorganic complexes



Large scale MOF screening



Sarah Peabody

Molecular pKa and
solvation entropy

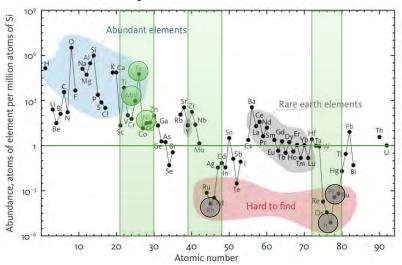


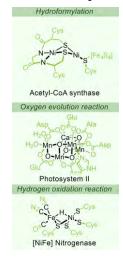
Fontillas
Structure-function relationships





Nature catalyzes "industrial" reactions using metalloenzymes



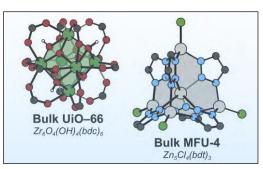


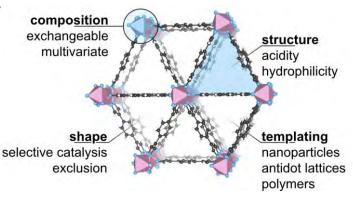
21

Metal-organic frameworks: static structures or dynamic crystals?

A useful family of materials. But they seem to vibrate and feature more local disorder than we first assumed.

Implications for catalysis and material stability





J. Am. Chem. Soc., 2020, 142, 19291

22



Apologies if there is a topic we don't have time for

American Chemical Society overview talk on coffee

ACS Webinar, "Coffee: A Chemical and Physical Perspective"
This is a "general-overview-of-coffee" talk, please check it out!

Re:Co talk on cooling coffee (green and roasted) came online

SCAA Symposium YouTube Channel, "Cryogenics: Facts and Fiction"

Tamper Tantrum on the physics of particle migrations Tamper Tantrum, "A Taste of Physics" — The Brazil Nut Effect

Water For Coffee 2.0

Establish Media, "Physical and Chemical Considerations in the Production of Coffee"



23



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Water For Coffee 2.0

Establish Media, "Physical and Chemical Considerations in the Production of Coffee"



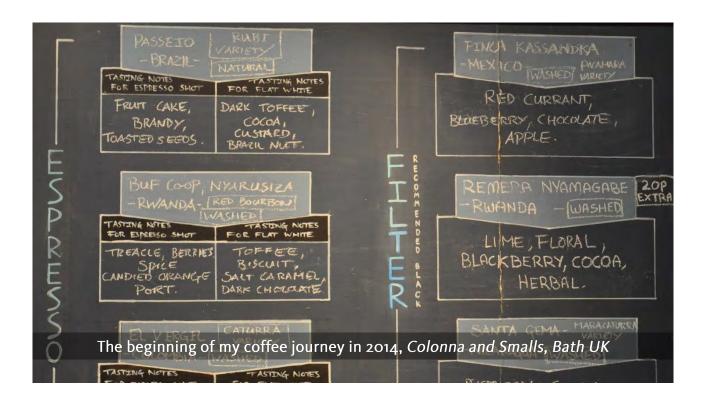
Trader Joes sells coffee

Note that there are not one plant...~10!



Coffee literature folder now hosted on pages . uoregon . edu / chendon / coffee_literature

1963 Tetrahedron, Diketone synthesis smokey flavors.pdf	23-Dec-2019 11:27 933K
1964 Tetrahedron, Volatiles in coffee,pdf	23-Dec-2019 11:27 1.0M
1968 Chem. Rev., Chemicals in tobacco and smoke,pdf	23-Dec-2019 18:07 6.3M
1979 Chem. Sens. Flavour, The misuse of "sour" and "bitter".pdf	23-Dec-2019 11:27 1.0M
1987 J. Appl. Bact., Effect of salt on growing bacteria.pdf	23-Dec-2019 19:12 777K
1988 Food Chem., Chemicals in blackberry juice.pdf	23-Dec-2019 11:27 321K
1990 J. Agric. Food Chem., Rio defect.pdf	23-Dec-2019 18:07 918K
1991 J. Sens. Stud., Chemistry of maple syrup.pdf	23-Dec-2019 11:27 848K
1992 Z. Lebensm. Unters. Forsch., Headspace freshness of roasted coffee.pdf	07-Jan-2020 22:10 597K
1995 Sens. Act. B, Sensors to sniff meat freshness.pdf	07-Jan-2020 22:10 446K







Audience Survey Question

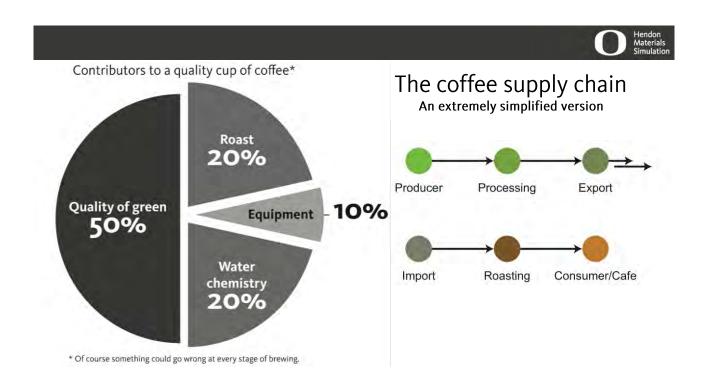
ANSWER THE QUESTION ON BLUE SCREEN IN ONE MOMENT

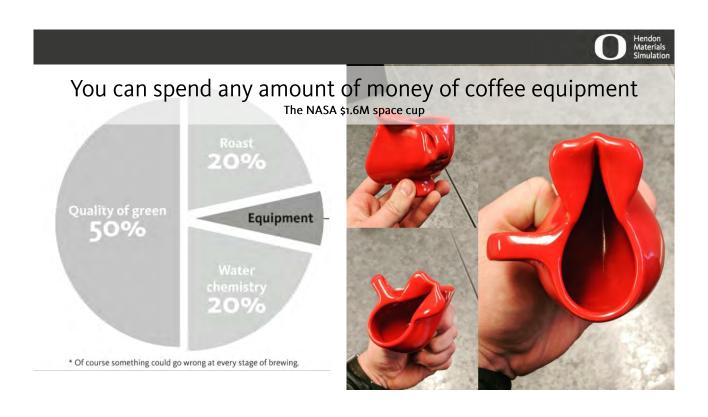


Which is the largest contributor to a quality cup of coffee?

- Roast
- · Water chemistry
- Equipment
- · Quality of the green
- Country of Origen



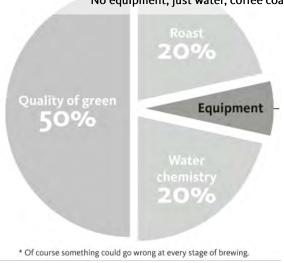




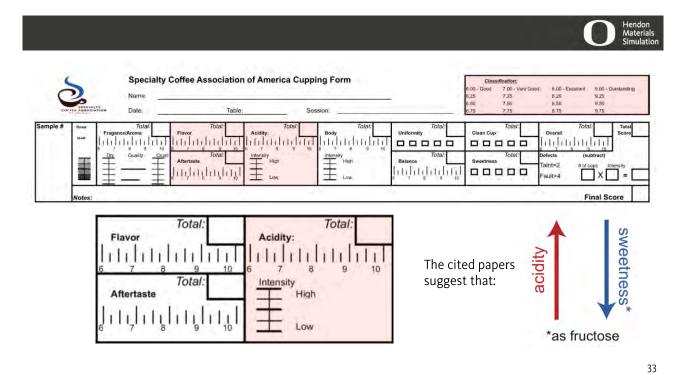


Coffee is graded on the cupping table

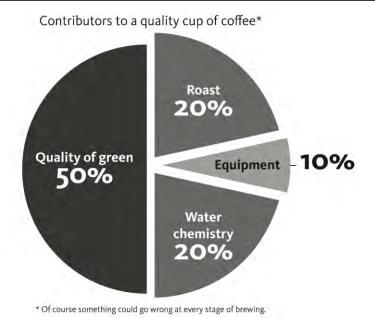
No equipment, just water, coffee coarsely ground, and a spoon + 4 min brew time



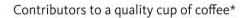


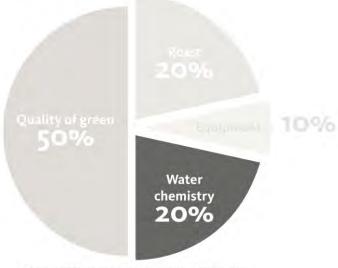












* Of course something could go wrong at every stage of brewing.

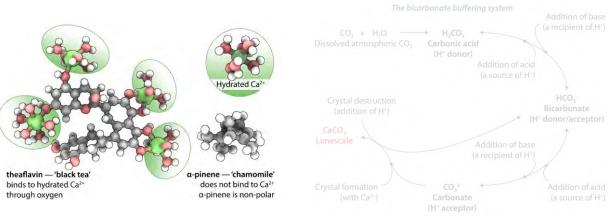


Water For Coffee Espresso?

Cations increase ionic strength of water

Cations (+) extract flavor

Anions (–) structure flavor



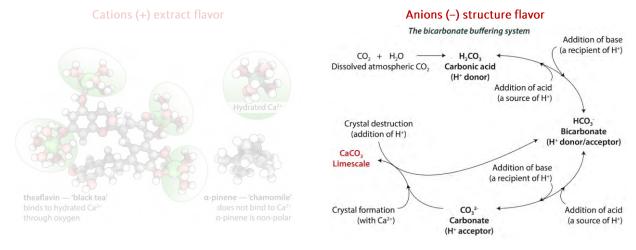
J. Agric. Food Chem., 2014, 62, 4947

Water For Coffee, 2021



Water For Coffee Espresso?

Buffers structure the perceived acids in coffee drinks

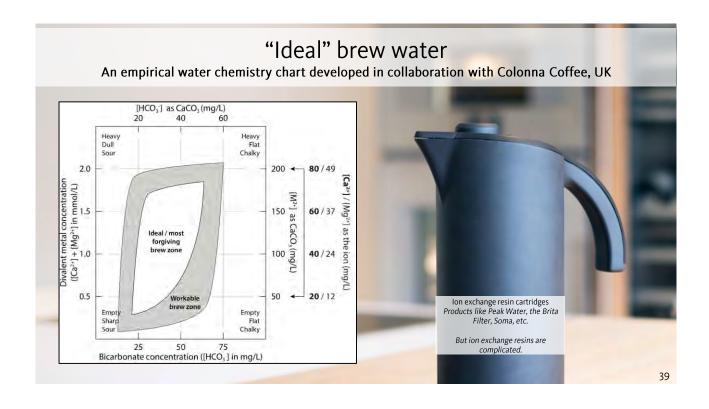


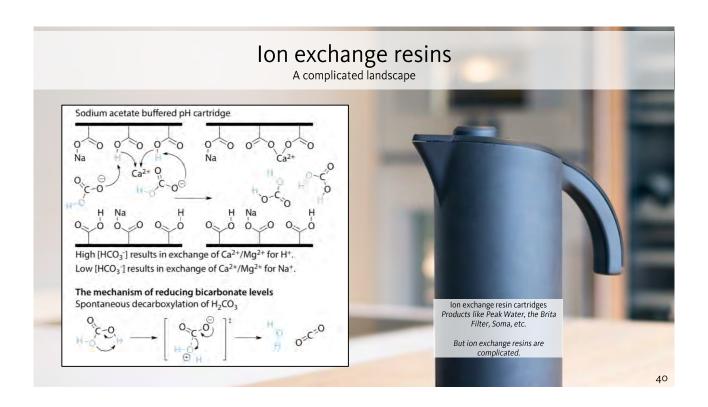
J. Agric. Food Chem., 2014, 62, 4947

Water For Coffee, 2021

37

(Positive) flavors in coffee are strongly affected by buffers Increasing bicarbonate concentration https://worldcoffeeresearch.org/work/sensory-lexicon/

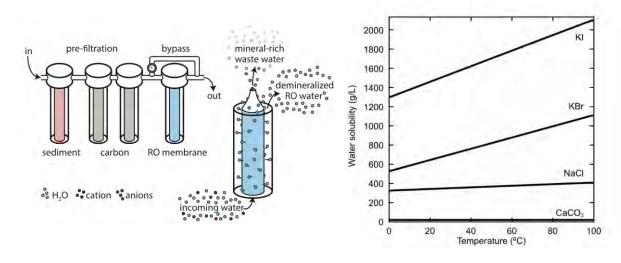






A comment on remineralization cartridges

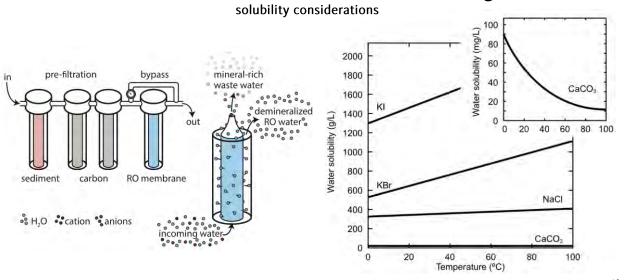
solubility considerations



41



A comment on remineralization cartridges





A thought on espresso vs. filter water let's consider water containing 50 mg/L HCO₃20% extraction from 20 g of coffee 4 g of solvated coffee stuff

Espresso Filter
40 mL water 400 mL water

VS.

43



A thought on espresso vs. filter water let's consider water containing 50 mg/L HCO₃20% extraction from 20 g of coffee 4 g of solvated coffee stuff

Espresso Filter
40 mL water HCO_3^- mass = 0.04 L * 50 mg2 mg of HCO_3^-



A thought on espresso vs. filter water let's consider water containing 50 mg/L HCO₃20% extraction from 20 g of coffee

4 g of solvated coffee stuff

Espresso		Filter
40 mL water		400 mL water
HCO_3^- mass =	VS.	HCO_3^- mass =
o.o4 L * 50 mg		o.4 L * 50 mg
2 mg of HCO_3^-		20 mg of HCO_3^-

45



A thought on espresso vs. filter water let's consider water containing 50 mg/L HCO₃20% extraction from 20 g of coffee 4 g of solvated coffee stuff

Espresso		Filter
40 mL water		400 mL water
HCO_3^- mass =	VS.	HCO_3^- mass =
o.o4 L * 50 mg		o.4 L * 50 mg
2 mg of HCO_3^-		20 mg of HCO_3^-

If you have hard water you should make smaller drinks ESPRESSO!





Extremely high
(quantitative)
extraction yield of
shikimic acid

Shikimic acid is a precursor to some anti-cancer drugs

Figure S1: Extraction of star anise using an espresso machine.



The definition of espresso

according to the Specialty Coffee Association

An espresso is a 25–35 mL (ca. 20–30 g) beverage prepared from 7–9 g of ground coffee made with water heated to 92 – 95 °C, forced through the granular bed under 9–10 bar of static water pressure and a total flow time of 20–30 s.

- Nobody really makes espresso any more
 - -Examples:
 - The Double Rizzi Banga Upwards of 26 g of coffee, producing a < 30 mL beverage
 - The Single Espresso Half of a shot prepared on an 18 20 g dose of coffee.



Espresso is more than just a ratio



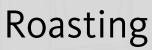
7 g basketTraditional "espresso" basketStepped.



15, 18, 20, 22 g baskets Modern "espresso" basket **Cylindrical**.

49

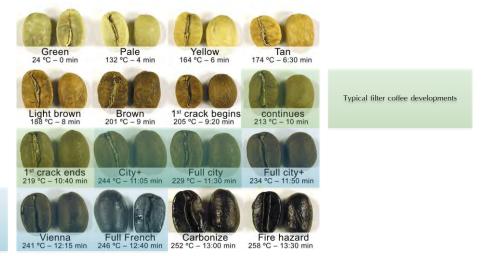






Espresso roasts are typically "darker"

higher pressure, short extraction times, a need to get more out of the coffee than just organic acids.



Typical espresso coffee developments

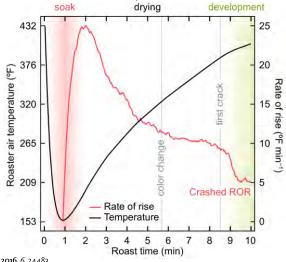
51



The roast profile

Kinetics: Gradient and time determine flavor development





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



Dark* roasted coffee is a good O₂ reduction catalyst *dark = 800 °C, ZnCl₂, Ar

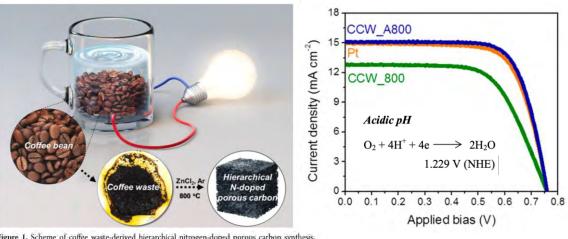
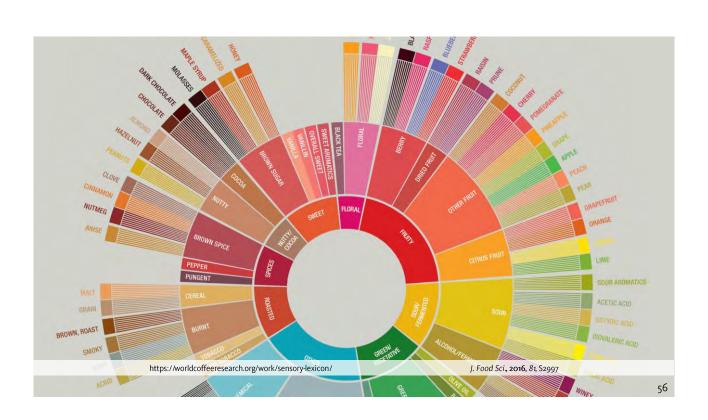


Figure 1. Scheme of coffee waste-derived hierarchical nitrogen-doped porous carbon synthesis.

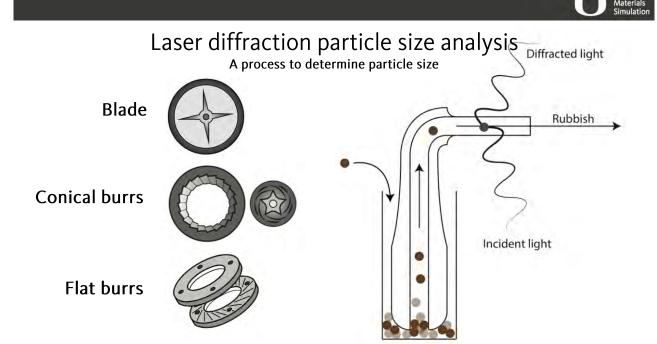
ACS. Appl. Mater. Interfaces, 2017, 9, 41303











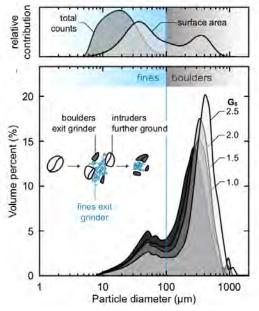


Laser Diffraction in Colonna and Smalls

Beckman Coulter lent us an instrument (and a guy to operate it) for a day







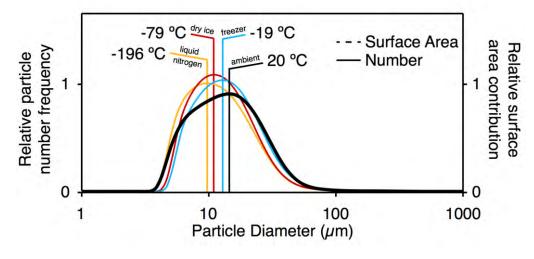
The effect of changing grind setting Grinding finer make more fine particulates, and small large particulates



Sci. Rep., 2016, 6, 24483



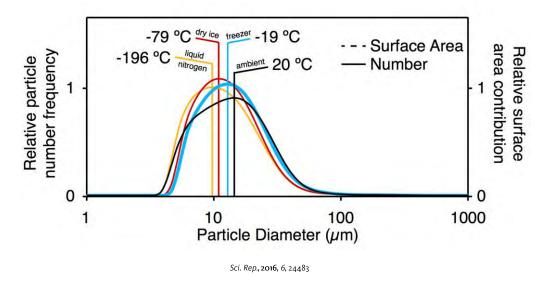
Cooling coffee before grinding augments the fine particle sizes



Sci. Rep., 2016, 6, 24483



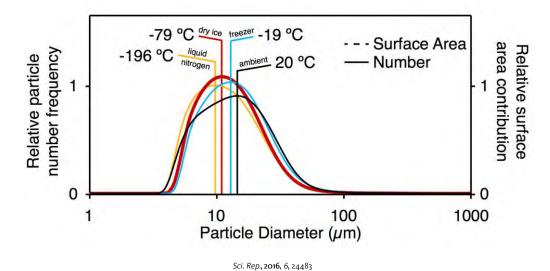
Cooling coffee before grinding augments the fine particle sizes



63

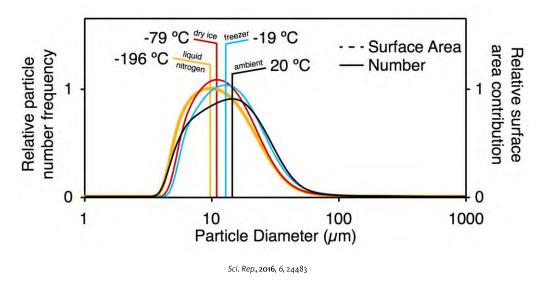


Cooling coffee before grinding augments the fine particle sizes





Cooling coffee before grinding augments the fine particle sizes

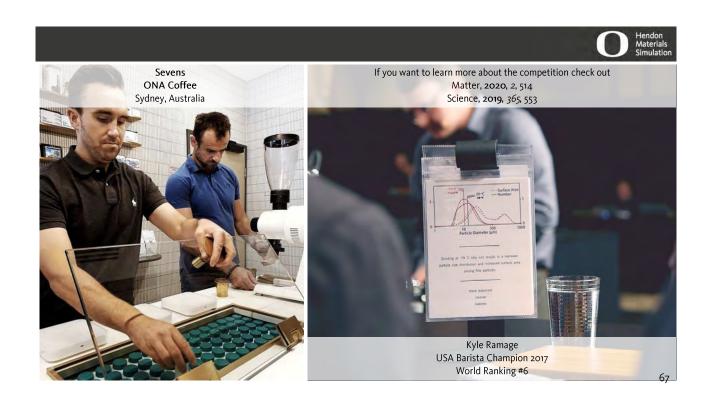


Hendon Materials Simulation

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Some cafes and coffee enthusiasts have adopted freezing coffee.

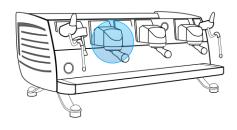


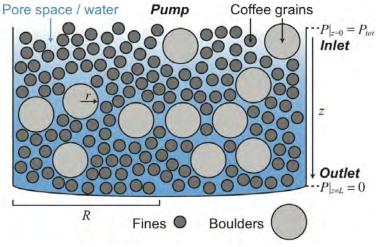






Development of a numerical model for extraction from a granular bed





Matter, 2020, 2, 63



Early studies of extraction and isolation of rates The exceptional work of Spiro

J. Sci. Food Agric: 1984, 35, 915-924

The Kinetics and Mechanism of Caffeine Infusion from Coffee: The Effect of Particle Size

Michael Spiro and Robert M. Selwood

J. Sci. Food Agric. 1984, 35, 925-930

The Kinetics and Mechanism of Caffeine Infusion from Coffee: Hydrodynamic Aspects

Michael Spiro and Caroline M. Page

J. Sci. Food Agric. 1985, 36, 871-876

The Kinetics and Mechanism of Caffeine Infusion from Coffee: the Effect of Roasting

Michael Spiro and Julia E. Hunter

J Sci Food Agric 1989, 46, 349-356

The Kinetics and Mechanism of Caffeine Infusion from Coffee: The Hindrance Factor in Intra-bean Diffusion

Michael Spiro, Ralf Toumi and Mangayetkarasy Kandiah

J Sci Food Agric 1993, 61, 371-373

Modelling the Aqueous Extraction of Soluble Substances from Ground Roast Coffee

Michael Spiro



The ongoing problem of quantifying what is extracted

 Brix-type measurement is used to quantify solvated mass. Works well for wine!

But for coffee?

TABLE 2

 $z = a + bx + cy + dx^2 + ey^2 + fxy$

wherein a = -7.27705E+02 b = -8.72678E-01 c = 5.46065E+02 d = 9.20185E-04 c = -4.68197E-01 f = 6.648126E-01 and x = temp y = nD z = % TDS



US Patent 8,239,144

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Extraction yield and total dissolved solids

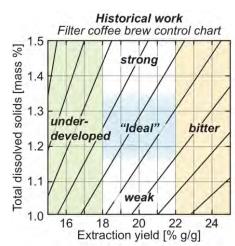
cumulative measurement of solvated mass

Extraction yield = Coffee mass solvated in the cup

Dry coffee mass used to brew

Total dissolved solids = Coffee mass solvated in the cup

Total mass of beverage





The refractive index of pure water at 25 °C

1.333

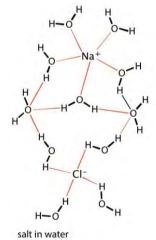
we are operating with very minor changes in refractive index.

74



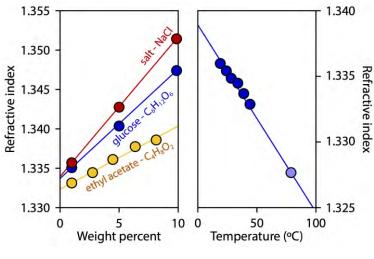
The refractive index is proportional to bulk liquid density

sugar in water





The refractive index is compound dependent!



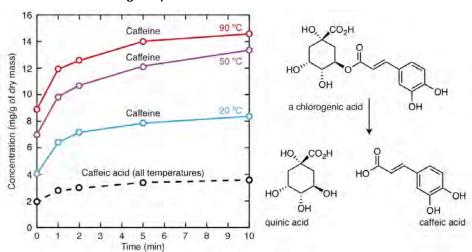
J. Chem. Eng. Data, 2015, 60, 2827

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Experimental kinetics

isolating temperature and molecular dissolution rates





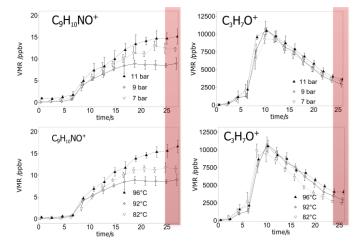
Kinetics of espresso extraction

A nice demonstration that the composition of a shot changes over time

Divide detectable compounds into families based on polarity

Both temperature and pressure change the composition of a shot at ~30s by ~50% for nonpolar things.

Less obvious for polar compounds.



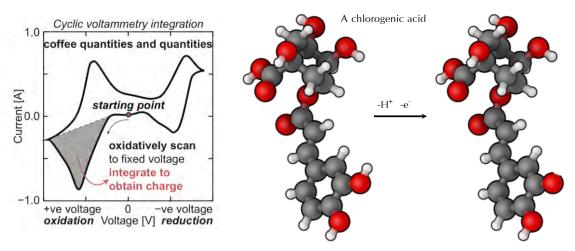
Int. J. Mass Spec., 2016, 401, 22

78



Our recently funded Coffee Science Foundation proposal

A proposal to move away from refractive index



Int. J. Electrochem. Sci., 2016, 11, 2854



Our recently funded Coffee Science Foundation proposal

A proposal to move away from refractive index

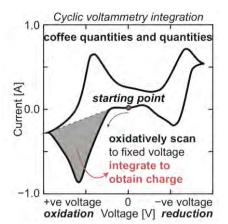


Table 2. Total chlorogenic acids (CGAs) content in different brand of coffees determined by DPV and HPLC methods

Brand of coffee	CGAs (total)-DPV ^a	CGAs (total)-HPLC ^b
C. Arabica, Rio Minas, Brazil (green bean)	7451	7370
C. Arabica, Rio Minas, Brazil (roasted bean)	2630	2613
C. Robusta, Cherry, India (green bean)	9115	9112
C. Robusta, Cherry, India (roasted bean)	2852	2826
Flatscher Olimpia (ground coffee, 100 % Arabica)	4101	3932
Franck Quatemala (ground coffee, 100 % Arabica)	3574	3519
Nescafé Classic (instant coffee)	3283	3203
Nescafé Espresso (instant coffee)	3229	3185
Jacobs Monarch (instant coffee)	3203	3149
Jacobs Intense (instant coffee)	3465	3462

Results represent mean value of three independent measurements (n=3)

Chlorogenic acid content is thought to contribute to

taste perception

Int. J. Electrochem. Sci., 2016, 11, 2854

80



Model parameterization

Most coffee professionals rely on a refractive index measurement that is then related to a coffee mass by some mathematical function

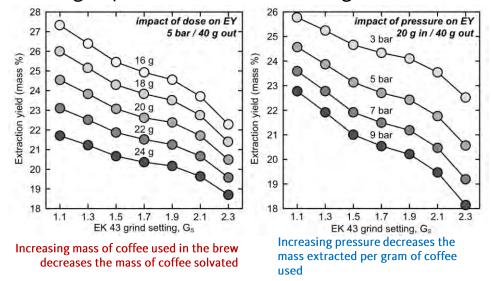
$$G = kc_s(c_s - c_l)(c_{sat} - c_l)$$
$$D_s = 6.25 \times 10^{-10} \text{m}^2/\text{s}, \quad k = 6 \times 10^{-7} \text{m}^7 \text{kg}^{-2} \text{s}^{-1}.$$

a-values determined by DPV, total CGAs content was expressed as 5-CQA equivalent (mg 5-CQAE/100 g of coffee)

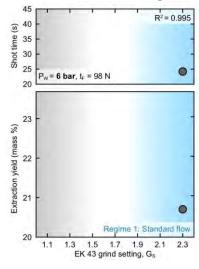
b- values determined by HPLC, total CGAs content were sum of individual CGAs content and expressed as mg CGAs/100 g of coffee



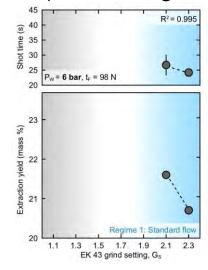
Predicting espresso extractions using relevant variables



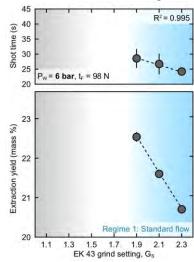




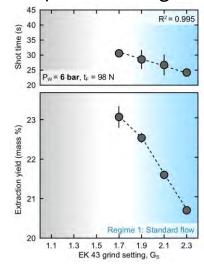




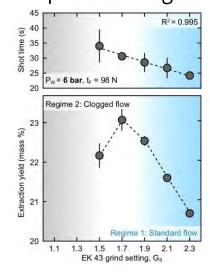




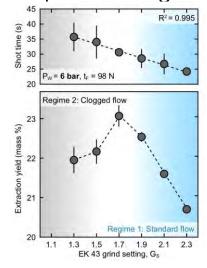




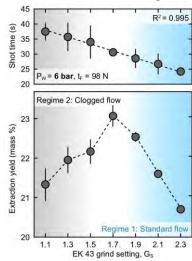




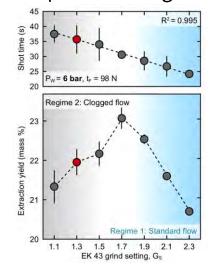




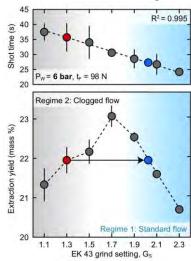




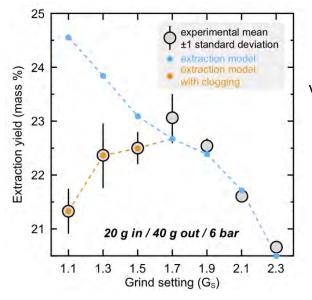










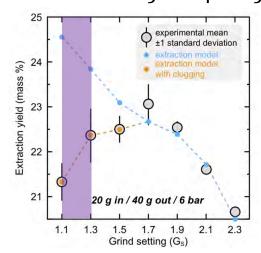


Volcano shape due to uneven contact of water to coffee particles in the bed.

"Channeling"



22%... a**25%+**b**24%+**c**23%...**n**15%...+**y**0%**

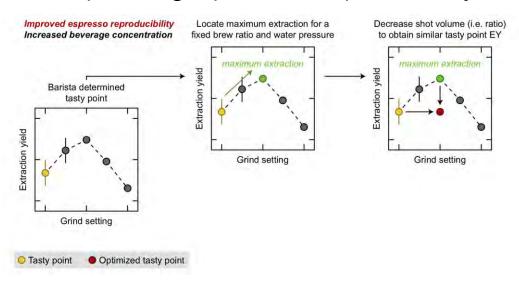


Critical populations on fines causing inhomogeneous extraction.

Grinder dependent, so you'll have to calibrate this yourself!

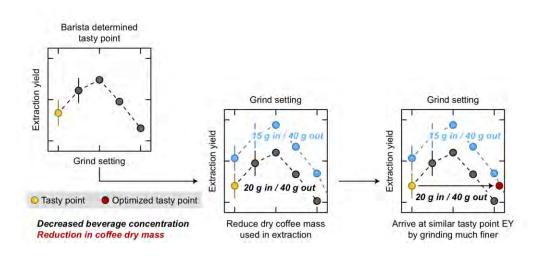


Optimizing espresso for reproducibility



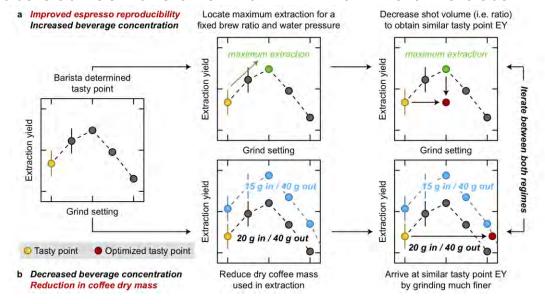


Optimizing espresso for reproducibility





Iterate between the two with minimum volume determined.





A case study of these turbo shots

Tailored Coffee Roasters, Eugene, OR

Shop sells 27,850 espresso drinks per year (a small store) Coffee wholesale value is \$26.4 /kg on average

20 g = \$0.528 of coffee dry mass 15 g = \$0.396 of coffee dry mass Savings per shot \$0.132

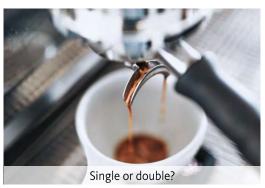
Total savings per year \$3,676 USD

Café that does 500 drinks per day (182,500 per year) saves \$24,000



Take home messages

- Espresso is a brew method, not a well-defined drink.
 - -The language of single and double espresso is convoluted by divergent paradigms in coffee brewing.





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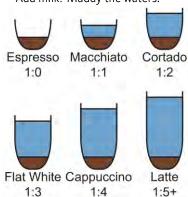


Take home messages

- Espresso is a brew method, not a well-defined drink.
 - -The language of single and double espresso is convoluted by divergent paradigms in coffee brewing.

 Add milk? Muddy the waters.







Take home messages

- Espresso is a brew method, not a well-defined drink.
 - The language of single and double espresso is convoluted by divergent paradigms in coffee brewing.
- Shot time depends on grind size and water pressure, and to a lesser extend coffee type and temperature.
 - Using time to quantify reproducibility is hence problematic, as it is one piece in a complex PDE.

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Take home messages

- Espresso is a brew method, not a well-defined drink.
 - The language of single and double espresso is convoluted by divergent paradigms in coffee brewing.
- Shot time depends on grind size and water pressure, and to a lesser extend coffee type and temperature.
 - Using time to quantify reproducibility is hence problematic, as it is one piece in a complex PDE.
- Kinetic experiments reveal that standard metrics for assessing "qualities" do not apply to espresso, or probably coffee in general.
 - Yet another use for electrochemistry?





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 MgSO₄.7H₂O (epsom salt)

~25 ppm Mg²⁺ as Mg²⁺

0.05 g/L NaHCO₃ (baking soda)

~35 ppm HCO₃ as HCO₃

Coffee preference: VERY APPROXIMATELY

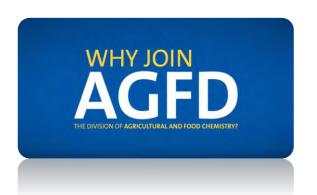
Acidic = East Africa (Kenya)

Chocolate and nuts = South/Central America (Brazil)

Low acid = Hawaii, India, Vietnam, Sumatra, and basically any "darker" roast

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Moderator: Daryl Boudreaux, Principal, Boudreaux & Associates LLC

- protection that have emerged in the United States over the past 200 years
- The challenges, limitations, and opportunities of more ontological
- approaches to the interpretation of water for public audiences Why museums and galleries should interpret water not as a singular
- material that preexists its understanding by scientific or indigenous knowledge, but rather as a multiplicity made by and bound up in systems of bodies, practice, power, and places

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- . Challenges in recycling of plastics and scaling new depolymerization
- Chemical pathways for breaking down single-use plastics with an emphasis on polyethylene
- . How food companies can modify their relationship towards plastics to face the public concerns linked to plastic packaging
- Mechanical recycling and its limitations and the emerging solutions for chemical recycling

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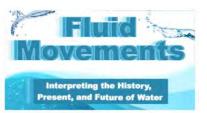
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