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Type them into questions box!

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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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Christopher Hendon
Assistant Professor, Department of Chemistry and Biochemistry, University of Oregon

Brian Guthrie
Corporate Research Fellow, Cargill

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Hendon
Materials
Simulation

Espresso Chemistry
From First Principles to Current Challenges

Prof. Christopher H. Hendon
Department of Chemistry and Biochemistry
University of Oregon

g chendon @ uoregon . edu — t
Bath, United Kingdom
Founded in 3

The Roman Baths
Hendon Materials Simulation — 2020

- Jenna Mancuso: Photoactive MOFs and chemical kinetics
- Austin Mroz: Machine learning and materials theory
- Khoa Le: Conductive MOFs
- Josh Davis: Water dissociation and solid/liquid interfaces
- Jack Yang: Molecular redox and inorganic complexes
- Lillian Payne: Large scale MOF screening
- Sarah Peabody: MolecularpKa and solvation entropy
- Natalie Fontillas: Structure-function relationships
Nature catalyzes “industrial” reactions using metalloenzymes

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

- 1979 Chem. Sens. Flavour. The misuse of "sour" and "bitter".pdf

The beginning of my coffee journey in 2014, Colonna and Smalls, Bath UK
The aim
reproducibly flavorsome coffee

The occasional outcome
something not so tasty
Which is the largest contributor to a quality cup of coffee?

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

Contributors to a quality cup of coffee*

* Of course something could go wrong at every stage of brewing.
You can spend any amount of money on coffee equipment

The NASA $1.6M space cup

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

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.
The cited papers suggest that:

*as fructose

Contributors to a quality cup of coffee*

- Quality of green: 50%
- Roast: 20%
- Water chemistry: 20%
- Equipment: 10%

* Of course something could go wrong at every stage of brewing.
Contributors to a quality cup of coffee*

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

---

Water For Coffee Espresso?
Cations increase ionic strength of water

Cations (+) extract flavor

- theaflavin — 'black tea' binds to hydrated Ca²⁺ through oxygen
- α-pinene — 'chamomile' does not bind to Ca²⁺, α-pinene is non-polar

Anions (-) structure flavor

- $\text{CO}_2 + \text{H}_2\text{O} \rightarrow \text{H}_2\text{CO}_3$ Carboxic acid (H⁺ donor)
- $\text{H}_2\text{CO}_3 \rightarrow \text{HCO}_3^-$ Bicarbonate (H⁺ donor/acceptor)
- Crystal formation (with Ca²⁺)
- $\text{CO}_3^{2-}$ Carbonate (H⁺ acceptor)
- Addition of base (a recipient of H⁺)
- Crystal destruction (addition of H⁺)
- Addition of acid (a source of H⁺)

The bicarbonate buffering system

---

Water For Coffee Espresso?
Buffers structure the perceived acids in coffee drinks

Cations (+) extract flavor

Anions (−) structure flavor

The bicarbonate buffering system

- Addition of base (a recipient of H⁺)
- Addition of acid (a source of H⁺)
- Addition of acid (a source of H⁺)
- Addition of base (a recipient of H⁺)
- CO₂⁻ Carbonate (H⁺ acceptor)
- HCO₃⁻ Bicarbonate (H⁺ donor/acceptor)
- H₂CO₃ Carbonic acid (H⁺ donor)
- CO₂ + H₂O Dissolved atmospheric CO₂

Crystal formation (with Ca²⁺)
Limescale
CaCO₃

Crystal destruction (addition of H⁺)
α-pinene — ‘chamomile’ does not bind to Ca²⁺
theaflavin — ‘black tea’ binds to hydrated Ca²⁺ through oxygen

(Positive) flavors in coffee are strongly affected by buffers

https://worldcoffeeresearch.org/work/sensorylexicon/

Water For Coffee, 2021

https://worldcoffeeresearch.org/work/sensorylexicon/

J. Food Sci., 2016, 81, 52997
“Ideal” brew water
An empirical water chemistry chart developed in collaboration with Colonna Coffee, UK

Ion exchange resins
A complicated landscape
A comment on remineralization cartridges
solubility considerations

A comment on remineralization cartridges
solubility considerations
A thought on espresso vs. filter water

let's consider water containing 50 mg/L $\text{HCO}_3^-$

20% extraction from 20 g of coffee

4 g of solvated coffee stuff

<table>
<thead>
<tr>
<th>Espresso</th>
<th>Filter</th>
</tr>
</thead>
<tbody>
<tr>
<td>40 mL water</td>
<td>400 mL water</td>
</tr>
</tbody>
</table>

VS.

<table>
<thead>
<tr>
<th>Espresso</th>
<th>Filter</th>
</tr>
</thead>
<tbody>
<tr>
<td>40 mL water</td>
<td>400 mL water</td>
</tr>
<tr>
<td>$\text{HCO}_3^-$ mass =</td>
<td>VS.</td>
</tr>
<tr>
<td>0.04 L * 50 mg</td>
<td></td>
</tr>
<tr>
<td>2 mg of $\text{HCO}_3^-$</td>
<td></td>
</tr>
</tbody>
</table>
A thought on espresso vs. filter water

let's consider water containing 50 mg/L HCO₃⁻

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<tr>
<td>40 mL water</td>
<td>400 mL water</td>
</tr>
<tr>
<td>HCO₃⁻ mass =</td>
<td>HCO₃⁻ mass =</td>
</tr>
<tr>
<td>0.04 L * 50 mg</td>
<td>0.4 L * 50 mg</td>
</tr>
<tr>
<td>2 mg of HCO₃⁻</td>
<td>20 mg of HCO₃⁻</td>
</tr>
</tbody>
</table>

If you have hard water you should make smaller drinks

ESPRESSO!
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 basket
   Traditional “espresso” basket
   Stepped.

15, 18, 20, 22 g baskets
   Modern “espresso” basket
   Cylindrical.

---

Roasting
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

The roast profile
Kinetics: Gradient and time determine flavor development


Sci. Rep. 2016, 6, 24481
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

https://worldcoffeeresearch.org/work/sensorylexicon/
J. Food Sci, 2016, 81, 52997
Grinding

whole bean  coarse  medium
Laser diffraction particle size analysis
A process to determine particle size

Blade
Conical burrs
Flat burrs

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 makes more fine particulates, and small large particulates

Cooling coffee before grinding augments the fine particle sizes
Cooling coffee before grinding augments the fine particle sizes

[Graph showing the effect of different cooling methods on particle size distribution]


63

Cooling coffee before grinding augments the fine particle sizes

[Graph showing the effect of different cooling methods on particle size distribution]


64
Cooling coffee before grinding augments the fine particle sizes.

Some cafes and coffee enthusiasts have adopted freezing coffee.
Sevens
ONA Coffee
Sydney, Australia

If you want to learn more about the competition check out
Matter, 2020, 2, 514
Science, 2019, 365 553

Kyle Ramage
USA Barista Champion 2017
World Ranking #6

Brewing
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

The Kinetics and Mechanism of Caffeine Infusion from Coffee: The Effect of Particle Size
Michael Spiro and Robert M. Selwood

The Kinetics and Mechanism of Caffeine Infusion from Coffee: Hydrodynamic Aspects
Michael Spiro and Caroline M. Page
J. Sci. Food Agric. 1985, 36, 671-676

The Kinetics and Mechanism of Caffeine Infusion from Coffee: the Effect of Roasting
Michael Spiro and Julia E. Hunter

The Kinetics and Mechanism of Caffeine Infusion from Coffee: The Hindrance Factor in Intra-bean Diffusion
Michael Spiro, Ralf Toumi and Mangayetkarasy Kandiah

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>
<thead>
<tr>
<th>TABLE 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>$z = a + bx + cy + dx^2 + cy^2 + fxy$</td>
</tr>
</tbody>
</table>

wherein:
- $a = -2.37759E+02$
- $b = -8.72678E+01$
- $c = 5.46063E+02$
- $d = 9.30185E+04$
- $e = -4.6815E+00$
- $f = 6.49812E-01$ and
- $x = \text{temp}$
- $y = \text{ill}$
- $z = \% \text{ TDS}$

**Extraction yield and total dissolved solids**

**cumulative measurement of solvated mass**

Extraction yield = \[\frac{\text{Coffee mass solvated in the cup}}{\text{Dry coffee mass used to brew}}\]

Total dissolved solids = \[\frac{\text{Coffee mass solvated in the cup}}{\text{Total mass of beverage}}\]
The refractive index of pure water at 25 °C

1.333

we are operating with very minor changes in refractive index.

The refractive index is proportional to bulk liquid density

shown in increasing density →

ethyl acetate in water
sugar in water
salt in water
The refractive index is compound dependent!

\[ J. \text{Chem. Eng. Data, 2015, 60, 2827} \]

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 non-polar things.

Less obvious for polar compounds.

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

Our recently funded Coffee Science Foundation proposal
A proposal to move away from refractive index

A chlorogenic acid

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

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

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

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

$^b$-values determined by HPLC, total CGAs content were sum of individual CGAs content and expressed as mg 5-CQA/100 g of coffee

Chlorogenic acid content is thought to contribute to taste perception

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

Model parameterization

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

\[ G = k c_s (c_s - c_l)(c_{sat} - c_l) \]

\[ D_s = 6.25 \times 10^{-10} \text{ m}^2/\text{s}, \quad k = 6 \times 10^{-7} \text{ m}^7 \text{ kg}^{-2} \text{ s}^{-1}. \]
Predicting espresso extractions using relevant variables

Increasing mass of coffee used in the brew decreases the mass of coffee solvated

Increasing pressure decreases the mass extracted per gram of coffee used

The curious problem of grinding finer
The curious problem of grinding finer
The curious problem of grinding finer
The curious problem of grinding finer
The curious problem of grinding finer

![Graph showing extraction yield and shot time for different EK 43 grind settings.](image)

Regime 1: Standard flow
Regime 2: Clogged flow

- Extraction yield (mass %)
- Shot time (s)

Parameters:
- $P_w = 6$ bar
- $y = 98$ N

- $R^2 = 0.995$
Volcano shape due to uneven contact of water to coffee particles in the bed.

“Channeling”

22%...

\[ a_{25\%} + b_{24\%} + c_{23\%} + \ldots + y_{15\%} + y_{0\%} \]

Critical populations on fines causing inhomogeneous extraction.

Grinder dependent, so you’ll have to calibrate this yourself!
Optimizing espresso for reproducibility

**Improved espresso reproducibility**

*Increased beverage concentration*

Barista determined tasty point

- Extraction yield vs. Grind setting

**Locate maximum extraction for a fixed brew ratio and water pressure**

- Maximum extraction

**Decrease shot volume (i.e. ratio) to obtain similar tasty point EY**

- Extraction yield vs. Grind setting

**Optimizing espresso for reproducibility**

**Decreased beverage concentration**

*Reduction in coffee dry mass*

Barista determined tasty point

- Extraction yield vs. Grind setting

**Reduce dry coffee mass used in extraction**

- Grind setting

- Extraction yield

**Arrive at similar tasty point EY by grinding much finer**

- Grind setting

- Extraction yield

- 15 g in / 40 g out

- 20 g in / 40 g out

- Optimized tasty point
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.
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?
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$_2$O (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 (Kenya)
**Chocolate and nuts** = South/Central America (Brazil)
**Low acid** = Hawaii, India, Vietnam, Sumatra, and basically any “darker” roast
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