**Dissolution Flow Instabilities in Coffee Brewing**

W. T. Lee, A. Smith, and A. Arshad

_School of Computing and Engineering, University of Huddersfield, Queensgate, Huddersfield HD1 3DH, UK._

(Dated: June 27, 2022)

A recent experiment showed that, contrary to theoretical predictions, beyond a cutoff point grinding coffee more finely results in lower extraction. One potential explanation for this is that fine grinding promotes nonuniform extraction in the coffee bed. We investigate the possibility that this could occur due to an instability involving dissolution and flow. A low dimensional model in which there are two possible pathways for flow is formulated and analysed. This model reproduces the qualitative trend observed due to combination of a flow instability and saturation of extraction in one pathway. This strongly suggests that a flow instability can explain the observed decrease in extraction.

Espresso coffee is a beverage brewed from the roasted, ground cherries (beans) of the coffee robusta or arabica plant. In brewing an espresso hot (92-95 °C) water is forced at high pressure (9-10 atmospheres) through a bed of 15-22 g of finely ground coffee resulting in a beverage with a mass of 30-60 g. Although coffee is a complex mix of nearly 2000 chemicals, most mathematical models of coffee brewing treat coffee as a single substance using mass as a measure of the amount. The quality of coffee can be measured by two properties: strength and extraction yield. Strength is the mass concentration of dissolved coffee solids in the beverage. Extraction yield is the mass fraction of the coffee grains that have dissolved. Coffee grains are only partially soluble so there is a maximal value of the extraction yield which can’t be exceeded. A rough measure of coffee quality is given by the coffee quality control chart which plots strength against extraction yield.

Fasano et al. developed a partial differential equation model of espresso brewing which treated coffee as a multicomponent substance. However, the primary interest of the authors was in the mathematical properties of the equations e.g., investigating the existence and uniqueness of solutions rather than parameterising the model with experimental data. Moroney et al. developed a multiscale model of cafetiere and filter coffee brewing based on models of groundwater flow and leaching. These models describe coffee as a dual porosity medium with pores between grains of ground coffee and pores within ground coffee. The model also included a bimodal size distribution of coffee grains. Cameron et al. developed a model of espresso brewing to investigate the effect of grain size on extraction and compared their results to experiment. Their approach is based on mathematical models of lithium ion batteries. Similarly to the models developed by Moroney et al. the model includes a bimodal grain size. A diffusion equation is used to model transport of coffee within grains to the intergranular pores. Smith and Lee developed a simplified model of coffee brewing for teaching purposes. This was applied to cafetiere brewing and only considered a single grain size.

Cameron et al.’s experiment looked at the trend of extraction yield with grind size parameterised by the setting of their grinder denoted by $g$. Small values of $g$ indicate finely ground coffee, whilst larger values of $g$ describe more coarsely ground coffee. Surprisingly a plot of extraction yield against grind size shows a peaked distribution with a maximum extraction at intermediate grind size values and less extraction seen for coarser and more finely ground coffee. This same trend of finer particles giving weaker coffee below a threshold value is also observed in other brewing methods. The expected trend was that extraction would increase as grind size decreased due to a combination of factors. These are: reduced permeability resulting in slower flow and thus liquid spending more time in contact with the coffee grains, a larger surface area over which transfer could occur and a smaller distance from the interior of the grains to the exterior. Thus in order to explain the observed deviation from the expected trend the authors hypothesised that at low grain sizes the entire coffee bed was not participating in extraction. In other words there was an increasing trend of extraction with grind size, but this was counter-balanced by a reduced volume of the coffee bed available for extraction. The mathematical model developed in the paper predicted the expected trend of increasing extraction with decreasing grind size. In order to agree with the observed trend a reduced area participating in extraction beyond the peak in extraction was imposed on the model. The authors speculated this might be due to fines clogging some pathways.

Here we consider the possibility that an instability linking flow and extraction may explain the experimental data. In this hypothesis the fluid has access to every area of the coffee bed, but flow and thus extraction proceeds more slowly in some regions than others. This proposed instability is based on a positive feedback loop in which flow and extraction reinforce each other. Extraction causes an increase in porosity and thus permeability. This increase in permeability will in turn lead to more flow and so more extraction will occur. This suggests that small differences in porosity in the coffee bed will become amplified over time. Regions with higher poros-
is the porosity of bed and dissolved coffee in the fluid passing through each bed; size is assumed to be time independent but a function of grind functions of time only not of any spatial variables. We neglect the vertical stratification of the coffee bed used fraction of each bed occupied by fluid. For simplicity we model that could show this behaviour would require two possible pathways along which flow and extraction could be different as shown in Figure 1. The key variables of this model are: \( Q_1 \) and \( Q_2 \), the volumetric flow rates through each bed; \( c_1 \) and \( c_2 \), the mass concentration of dissolved coffee in the fluid passing through each bed; and \( \epsilon_1 \) and \( \epsilon_2 \), the porosity of each bed, i.e. the volume fraction of each bed occupied by fluid. For simplicity we neglect the vertical stratification of the coffee bed used in previous models. Thus the variables of the model are functions of time only not of any spatial variables.

The total flow rate, \( Q = Q_1 + Q_2 \), through the system is assumed to be time independent but a function of grind size \( q \). It is estimated as \( Q = M_{\text{shot}}/\rho_{\text{w}} t_{\text{shot}} \). (We follow Ref. [6] in assuming that the fluid volume is unaffected by dissolved coffee content.) To find the flow rates through the individual pathways we use the Kozeny–Carman equation for the permeability of a porous medium of spherical particles [4] to relate porosity to permeability and thus flow resistance. Flow through each pathway is given by

\[
Q_{1,2} = \frac{Q \kappa_{1,2}}{\kappa_1 + \kappa_2},
\]

\[
\kappa_{1,2} = \frac{\epsilon_{1,2}^3}{1 - \epsilon_{1,2}^2},
\]

where \( \kappa_i \) is a dimensionless permeability of bed \( i \) and \( \epsilon_i \) is the porosity of bed \( i \) (\( i = 1, 2 \)).

Extraction is modelled following Moroney [6]. The transfer rate of transfer of coffee from the grains into the fluid is given by \( SD(c_{\text{sat}} - c)/\lambda \) where \( S \) is the surface area of grains, \( D \) is the diffusivity, \( c_{\text{sat}} \) is the concentration at the surface of the grains, assumed to be saturated, \( c \) is the mass concentration of dissolved coffee solids in the liquid and \( \lambda \) is a diffusion length. Using a single term to describe transfer between the solid and the liquid implicitly assumes that the distribution of ground coffee is unimodal. (The same assumption underlies using the Kozeny–Carman equation for permeability also.) In fact coffee grain size distributions are better modelled as bimodal, but we follow Ref. [13] in only considering a single transfer term for simplicity. To relate extraction to changes in porosity we assume that the soluble and insoluble components of coffee have the same density. This also allows us to relate extraction yield to porosity via

\[
EY(t) = \frac{\epsilon(t) - \epsilon(0)}{1 - \epsilon(0)},
\]

where \( EY(t) \) is extraction yield and \( \epsilon(t) \) is the porosity at time \( t \).

Flow instabilities in reacting porous media have been studied using continuum [11] and microcontinuum methods [14, 15]. In both approaches instability is investigated by direct simulation. We thus include a small difference \( \delta \) in the porosities of the coffee beds in pathways 1 and 2, taking \( \epsilon_{1,2} = \epsilon_0 \pm \delta \) at \( t = 0 \). To see if there is an instability we simply simulate the evolution of the system and observe whether the difference in porosity grows or shrinks over time. To solve the differential equations we use a 4th order Runge-Kutta method with adaptive time stepping [12]. To determine the parameters \( D/\lambda, \delta \) and \( EY_{\text{max}} \) we use least squares fitting comparing simulated extraction yields to the data. To do this we form a sum of squares:

\[
\chi^2(D/\lambda, \delta, EY_{\text{max}}) = \sum_i (EY_{\text{model},i} - EY_{\text{data},i})^2.
\]

Constrained BFGS [10] minimisation of this function is used to find optimal values of the parameters.

From the considerations above the differential equations describing conservation of coffee in the solid grains and in the liquid are

\[
\frac{d}{dt} \left( \frac{\epsilon_i ALC_i}{2} \right) = \frac{DS(c_{\text{sat}} - c_i)}{2\lambda} \theta_i - Q_i c_i,
\]

\[
\frac{d}{dt} \left[ \frac{(1 - \epsilon_i) ALC_i}{2} \right] = -\frac{DS(c_{\text{sat}} - c_i)}{2\lambda} \theta_i,
\]

\[
\theta_i = \begin{cases} 1 & \text{if } EY_i < EY_{\text{max}} \\ 0 & \text{otherwise,} \end{cases}
\]

where \( \theta_i \) is an indicator function showing whether any soluble coffee remain in the coffee grains. Initial conditions are \( c_{1,2} = 0 \) and \( \epsilon_{1,2} = \epsilon_0 \pm \delta \).
FIG. 2. Linear fit to $t_{\text{shot}}$ the time taken to pour a shot vs the grind size setting $g$.

FIG. 3. Linear fit to $S$ the surface area of grains in the coffee bed vs the grind size setting $g$.

FIG. 4. Points show experimental data for Extraction yield, $EY$ as a function of grind size setting, $g$. The line shows the overall extraction yield from the best fit two pathway model. The model reproduces the qualitative trend.

The equations can be rearranged and nondimensionalised to the form

\[ \frac{d\epsilon_i}{d\tau} = (1 - C_i) \theta_i, \]

\[ \alpha \frac{dC_i}{d\tau} = (1 - C_i)(1 - \alpha C_i) \theta_i - \frac{2\alpha \beta \kappa_i}{\kappa_1 + \kappa_2} C_i, \]

where $C_i$ is a dimensionless concentration and $\tau$ is a dimensionless time derived from the scalings

\[ c_i = c_{\text{sat}} C_i, \]

\[ t = \frac{AL\rho_c \lambda}{Dc_{\text{sat}}} \tau. \]

The dimensionless parameters $\alpha$ and $\beta$ are given by

\[ \alpha = \frac{c_{\text{sat}}}{\rho_c}, \]

\[ \beta = \frac{Q\lambda}{DS}. \]

The time it takes to find pour a shot, $t_{\text{shot}}$, is needed to find $Q$. An expression for $t_{\text{shot}}$ in terms of grind size setting $g$ is determined by a linear fit to data in Ref. [1]. Figure 2 shows this results in a good fit to the data. Similarly the total surface area of grains in the coffee bed, $S$, needed for the dimensionless parameter $\beta$ is found by combining data on surface areas of large and small coffee grains in Ref [1] and then performing linear regression against grind size as shown in Figure 3.

Plotting the best fit model against the data, as seen in Figure 4 shows that although the two pathway model is very simple it can reproduce the qualitative features of the data, including decreasing extraction yield with decreasing grind size. Figure 5 shows the extraction yield from the individual pathways. The plot suggests that the transition from the expected behaviour of extraction increasing as grind size decreased to the surprising behaviour of decreasing extraction with decreasing grind size corresponds to the onset of saturation of extraction yield in one of the pathways i.e. to the dissolution of all available soluble coffee.

To see how extraction varies with time we show time dependent results from the two extreme grind sizes $g = 1.1$ and $g = 2.3$. The plot for finely ground coffee, $g = 1.1$, Figure 6 shows clearly that one pathway hits saturation point. For the coarsely grind sample, $g = 2.3$, Figure 7 shows the instability, but no saturation.

The parameters used in this model including those determined by fitting are shown in Table I. The dimen-
FIG. 5. Points show experimental data for Extraction yield, \(EY\) as a function of grind size setting, \(g\). The two lines show the extraction yield of the individual pathways from the best fit two pathway model.

FIG. 6. Porosity and dimensionless concentration of dissolved coffee solids as a function of dimensionless time for finely ground coffee. All the soluble coffee is extracted from bed 1 at \(\tau \approx 0.8\).

FIG. 7. Porosity and dimensionless concentration of dissolved coffee solids as a function of dimensionless time for coarsely ground coffee.

TABLE I. Parameter values used in simulations and their sources. In the case of \(\rho_c\) both the value from the literature and the unphysical value used here are reported.

| Parameter | Value | Source |
|-----------|-------|--------|
| \(\hat{M}_{\text{shot}}\) | 0.04 kg | Ref. [1] |
| \(\rho_w\) | 997 kg m\(^{-3}\) | Ref. [1] |
| \(\epsilon_0\) | 0.173 | Ref. [1] |
| \(c_{\text{sat}}\) | 212.4 kg m\(^{-3}\) | Ref. [1] |
| \(\rho_c\) | 399 kg m\(^{-3}\) | Ref. [1] |
| \(\rho_c\) | 798 kg m\(^{-3}\) | Imposed |
| \(\alpha\) | 3.76 | Calculated |
| \(\lambda/D\) | \(0.125 \times 10^6\) s m\(^{-1}\) | Best fit |
| \(\delta\) | 0.035 | Best fit |
| \(EY_{\text{max}}\) | 33.8 % | Best fit |

Porosity. This may be a result of the simplicity of the model.

In [1] an alternative but related explanation if proposed for the observed trends, namely that at smaller grind sizes clogging appears. In other words some pathways through the coffee bed are blocked by fines. Within this modelling framework this hypothesis would be supported by a large initial value of delta. There is thus some support for this within the model. However, the same value of delta is used for all the simulations, so the model does not support the idea that the onset of clogging is responsible for the turnover in the trend.

One unsatisfactory feature of the model is that the decreasing trend in extraction with grind size is not seen with the value of \(\rho_c\) observed experimentally in Ref. [1]. If this value is used then the extraction yield remains constant below the critical grind size but does not decrease. In order to see the observed behaviour of decreasing extraction with decreasing grind size an unphysical value of \(\rho_c\) twice the size of the physical value is used here. (Both
values for $\rho_c$ are given in Table[1] Given how simple the model is, it is not surprising that some adjustments of parameters must be made to reproduce the observed behaviour. In particular the large value of $\rho_c$ needed may indicate that including a bimodal size distribution may be needed.

These results also have implications for the taste of coffee. As is shown by the coffee brewing control chart over-extraction of coffee results in an excess of bitter flavours. Thus given that beyond the turnover point we expect at least some part of the coffee bed to be significantly over extracted, in fact for all soluble compounds to be dissolved, we would expect the coffee brewed beyond this point to have a more bitter taste than coffee brewed with the same overall extraction yield at the higher grind size.

The aim of this study was to investigate whether a flow instability could explain the anomalous trend of extraction yield with grind size seen experimentally by Cameron et al. [1]. The proposed instability was a positive feedback loop between flow and extraction. We investigated this in the simplest possible model capable of showing such an instability, one in which there were two potential pathways for flow. The instability was investigated by simulating the evolution of the system with an initial difference in porosity between the two pathways built in. Model parameters were either taken from the original paper, determined by curve fitting or in one case chosen in order to see the desired behaviour. Surprisingly for such a simple model the observed trend of a peak in extraction yield with grind size was reproduced.

In building this model the initial assumption was that the peak in extraction yield would indicate the onset of instability. In fact the model suggests that instability is always present and that the peak in extraction yield is due to saturation. In other words instability is always present but as the amount of coffee extracted from one region decreases, an overcompensating increase in the extraction of coffee from other regions masks this trend until all the soluble coffee is dissolved. This has important implications for the taste of the coffee, the non uniform extraction suggests that the average extraction yield may not be a good guide to taste particularly at fine grind sizes. This result also has implications for simulations of coffee brewing. These have typically focused on variations with depth but have not considered lateral variations in extraction.

A number of extensions to the model are possible which may result in a better fit to the observed data and may remove the need to incorporate an unphysical parameter value i.e. taking $\rho_c$ to be twice the size of the measured value. One example would be to include a bimodal description of the coffee grains. It is possible that the large value of $\rho_c$ is needed to compensate for the model not including the densely packed fine grains. Another feature that could be included that is already part of existing models is to include vertical stratification. The model currently assumes that porosity, and dissolved coffee concentration is uniform across the depth of the coffee bed. Relaxing this assumption would make the model more realistic as simulations show there is significant variation with depth. A final improvement to the model would be to remove the assumption that there are two equally weighted pathways for flow. This could be done either by including a larger number of pathways or by allowing the areas of the pathways to be different fractions of the total cross sectional area - this split could be included as one of the fitting parameters of the model.

This work suggests that if the instability in the flow could be eliminated or reduced then the taste of espresso coffee could be improved and significant financial and environmental costs associated with wasted material could be eliminated. One obvious thing to check first would be to make sure that flow was as even as possible. Depending on the exact nature of the instability it may be possible to prevent it by changing the aspect ratio of the coffee bed. If there is a macroscopic sized lateral length-scale associated with the instability then the instability could be eliminated by reducing the horizontal size of the coffee bed to make it smaller than the scale of the instability.

---

1. M. I. Cameron, D. Morisco, D. Hofstetter, E. Uman, J. Wilkinson, Z. C. Kennedy, S. A. Fontenot, W. T. Lee, C. H. Hendon, and J. M. Foster. Systematically improving espresso: Insights from mathematical modeling and experiment. *Matter*, 2(3):631–648, 2020.
2. N. Cordoba, L. Pataquiva, C. Osorio, F. L. M. Moreno, and R. Y. Ruiz. Effect of grinding, extraction time and...
type of coffee on the physicochemical and flavour characteristics of cold brew coffee. *Scientific reports*, 9(1):1–12, 2019.

[3] A. Fasano and F. Talamucci. A comprehensive mathematical model for a multispecies flow through ground coffee. *SIAM Journal on Mathematical Analysis*, 31(2):251–273, 2000.

[4] R. Holdich. *Fundamentals of particle technology*. MidlandIT, 2020.

[5] J. Melrose, B. Roman-Corrochano, M. Montoya-Guerra, and S. Bakalis. Toward a new brewing control chart for the 21st century. *Journal of agricultural and food chemistry*, 66(21):5301–5309, 2018.

[6] K. M. Moroney, W. T. Lee, S. B. G. O’Brien, F. Suijver, and J. Marra. Modelling of coffee extraction during brewing using multiscale methods: An experimentally validated model. *Chemical Engineering Science*, 137:216–234, 2015.

[7] K. M. Moroney, W. T. Lee, S. B. G. O’Brien, F. Suijver, and J. Marra. Asymptotic analysis of the dominant mechanisms in the coffee extraction process. *SIAM Journal on Applied Mathematics*, 76(6):2196–2217, 2016.

[8] K. M. Moroney, W. T. Lee, S. B. G. O’Brien, F. Suijver, and J. Marra. Coffee extraction kinetics in a well mixed system. *Journal of Mathematics in Industry*, 7(1):1–19, 2016.

[9] K. M. Moroney, K. O’Connell, P. Meikle-Janney, S. B. G. O’Brien, G. M. Walker, and W. T. Lee. Analysing extraction uniformity from porous coffee beds using mathematical modelling and computational fluid dynamics approaches. *PloS one*, 14(7), 2019.

[10] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery. *Numerical recipes 3rd edition: The art of scientific computing*. Cambridge university press, 2007.

[11] D. W. Rees-Jones and R. F. Katz. Reaction-infiltration instability in a compacting porous medium. *Journal of Fluid Mechanics*, 852:5–36, 2018.

[12] L. F. Shampine and M. W. Reichelt. The matlab ode suite. *SIAM journal on scientific computing*, 18(1):1–22, 1997.

[13] A. Smith and W. T. Lee. Brewing optimal coffee. *European Journal of Physics*, 42(2):025805, 2021.

[14] C. Soulaine, S. Roman, A. Kovscek, and H. A. Tchelepi. Mineral dissolution and wormholing from a pore-scale perspective. *Journal of Fluid Mechanics*, 827:457–483, 2017.

[15] C. Soulaine, S. Roman, A. Kovscek, and H. A. Tchelepi. Pore-scale modelling of multiphase reactive flow: Application to mineral dissolution with production of. *Journal of Fluid Mechanics*, 855:616–645, 2018.