MTM (Mass Transfer Matrix) Espresso extraction model

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This document describes an espresso extraction model which is influenced by the work presented in [1] and [2]. The model uses the coffee flow data collected during the espresso shot and the grind parameters along with other assumptions to predict the TDS (total dissolved solids) in the coffee drink. The model needs to be calibrated first to the TDS measurement data.

The main differences of this model compared to [2] is that a) this model uses directly the coffee flow data (which can be collected with e.g. Bluetooth scale) instead of trying to simulate it. This improves the accuracy of the model. And b) that the model uses natural discretisation of the coffee grains into "cells" to model the extraction dynamics, instead of using partial differential equations which are then discretised for numerical solution. With this approach the particle size distribution can be used directly to create families of grains with different sizes. This improves the accuracy of the model further.

The model is implemented in C# https://github.com/AndyZap/EspMod and is designed to work with DE1 espresso machine shot files.

References

1. K. M. Moroney, Heat and mass transfer in dispersed two-phase flows, Ph.D. thesis, University of Limerick (2016). https://ulir.ul.ie/handle/10344/6592
2. M. Cameron, D. Morisco, D. Hofstetter, E. Uman, J. Wilkinson, Z. Kennedy, S. Fontenot, W. Lee, C. Hendon, J. Foster, Systematically Improving Espresso: Insights from Mathematical Modelling and Experiment. Matter 2, 1–18 March 4, 2020, https://doi.org/10.1016/j.matt.2019.12.019

Possible use of the model

The coffee TDS measurements are common in assisting the search to a good brew recipe. The modern coffee brewing methods involves considerable range of the brew ratio, pressure and flow profiles. The TDS values obtained by different methods might be difficult to relate to each other. An espresso extraction model could tell if the differences are "the first order" effects, predictable by the model, or something more complicated (and possible undesirable) is going on – e.g. like channelling.

Model description

Following [1] and [2], we consider water flow through a cylindrical packed coffee bed (the puck).

A grinder breaks coffee beans into grains. For an espresso grind, a typical grain size is about 200-300 µm. An interesting feature of coffee grains is that they are composed from a little hollow cells with

size around 20-50 µm. In addition to the larger grains (the boulders), an espresso grind contains "fines" – small particles about the size of a coffee cell. These are usually the broken cell fragments.

A good grinder usually produces about 10-15% of fines from the total grind mass/volume. Also the particle size distribution of the boulders is rather narrow, i.e. dominated by grains of a particular size. Check [1] and [2] for typical particle size distributions graphs.

Figure 1 shows a schematic representation of a coffee bed. For simplicity, we model the coffee cells and the coffee grains as spheres. All coffee cells are of the same size. Following this assumption, the grains can only be composed of a certain number of cell layers, and the grain diameter can only take a set of discrete values: 1 cell diameter for 1 cell layer (=1 cell), 3 cell diameters for 2 cell layers, 5 cell diameters for 3 cell layers, etc (see the figure).

The space between grains is easily accessible by water. This is the path the water takes during the espresso extraction. Reference [1] suggests that the grains occupy about 83% of the puck volume, so the remaining 17% is the space between grains.

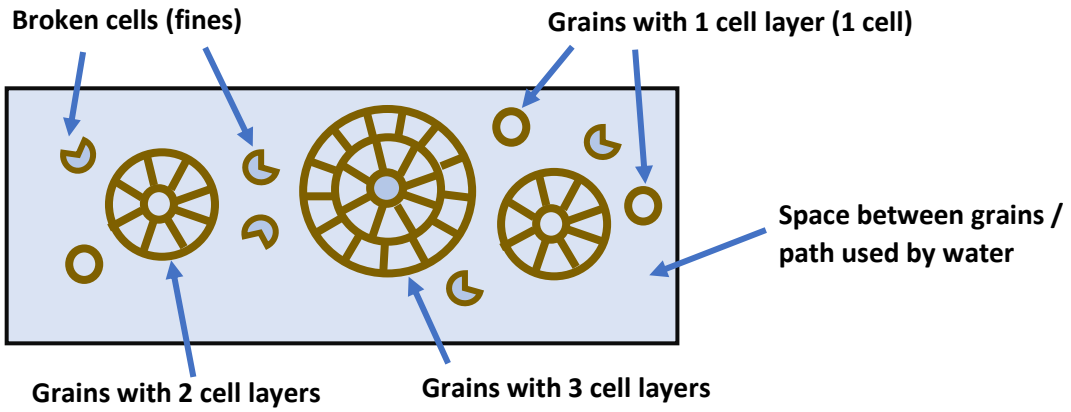

Figure 1. Schematic representation of a coffee bed as grains of different sizes.

At the beginning of the espresso extraction the puck is filled with water (the pre-infusion stage). The water fills not only the space between grains, but also the space inside the coffee cells due to the numerous micro-cracks created during the roasting process. [1] estimates that the volume inside cells is about 64% of the total grains volume. So from the total puck volume we have about 17% water volume between the grains and 83%*64%=53% inside the grains. The remaining volume is occupied by the coffee solids. Here we assume that these is no space between cells inside a grain, i.e. cells are packed next to each other.

Next let us turn to the part of the coffee grains which is soluble by water. It is estimated that about 30% of the ground coffee mass is soluble. What interesting, is that the soluble part dissolves in water rather quickly - in a few seconds. This means that the soluble mass in the broken cells / fines quickly dissolves into the water volume between grains.

It needs to be noted that the soluble part actually contains around 2,000 different compounds extracted from coffee grounds during brewing. But following [1] and [2], we model the total soluble coffee mass dynamics as some average quantity. The model could be rewritten to work with individual compounds, but such model would be difficult to calibrate to experimental data, as it difficult to measure the amount of an individual compound in the coffee brew. From the other hand,

the total dissolved solids (TDS) can be easily measured with a coffee refractometer, so a model formulated for the total soluble coffee mass can be calibrated without any difficulties.

Diffusion through the cell boundaries

The soluble coffee part inside cells dissolves quickly as well. But it is far more difficult for the coffee molecules to migrate into the space between grains where they could be picked by the moving water. This is a diffusion process and can be described using Fick's first law of diffusion: https://en.wikipedia.org/wiki/Fick%27s_laws_of_diffusion#Fick's_first_law. The law says that the speed of the mass transfer across the cell boundary (e.g. in gram per second) is proportional to the difference in the coffee mass concentration (e.g. in gram per mm^3) on both sides of the boundary.

For the mass transfer between two cells the formula can be written as:

$$dm = K^* \cdot (c_1 - c_2) \cdot dt = K^* \cdot \left(\frac{m_1}{V_{cell}} - \frac{m_2}{V_{cell}}\right) \cdot dt \quad (1)$$

Here dm is the amount of mass transferred over the cell boundary during the time interval dt, m_1 and m_2, c_1 and c_2 is the soluble coffee mass and the coffee concentration inside cell 1 and cell 2 correspondingly. V_{cell} is the void volume inside coffee cell which contains water and soluble coffee mass. K^* is a coefficient which describes the rate of diffusion between two cells. It is proportional to the diffusion coefficient and the area of the cell boundary, as they appear in the Fick's formula. As we assume that all cells are of the same size, we do not introduce a variable for the area of the cell boundary, and simply include it implicitly in the value of K^*.

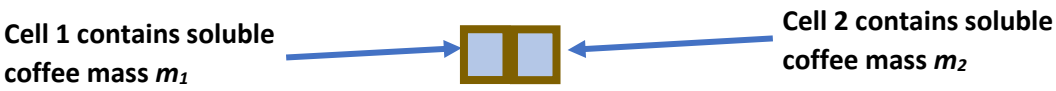

Figure 2. Diffusion mass transfer between two coffee cells

Instead of the coefficient K^* it is actually easier to work with another coefficient which is scaled by the void volume inside cell V_{cell}:

$$K^* = K \cdot V_{cell} \quad (2)$$

The equation (1) can now be rewritten as:

$$dm = K \cdot (m_1 - m_2) \cdot dt \quad (3)$$

K is the only coefficient used by the model which needs to be fitted to the experimental TDS measurements.

With dt=1 (second) and $K = 0.5$ we can see that the mass transferred over the boundary is equal to the half of the mass difference. I.e. after 1 second time step the mass in cells 1 and 2 become equal, so the diffusion process is complete. From the coffee brewing we know that it takes tens of seconds to extract coffee, so we might expect K values about 10 times smaller. So with the equation 3 we can easily estimate the values for the K coefficient which we expect from the model.

Next let us write the formula for the diffusion between a coffee cell and the space between coffee grains. This is the final destination of the diffusion process, where the soluble mass can be carried to the cup by moving water. Here we assume that the interface area in this case is about the same size as between two cell, so we use the same coefficient:

$$dm = K \cdot V_{cell} \cdot (c_1 - c_{between}) \cdot dt = K \cdot V_{cell} \cdot \left(\frac{m_1}{V_{cell}} - \frac{m_{between}}{V_{between}}\right) \cdot dt \quad (4)$$

Here we introduces new variables: $c_{between}$ and $m_{between}$ is the concentration and the soluble coffee mass in the space between grains, $V_{between}$ is the volume between grains.

Tracking the coffee mass changes in the cells during extraction

Clearly tracking soluble coffee mass in every coffee cell would make the model difficult to solve numerically, as the number of cells in a typical espresso puck is very large. Let us make some assumptions to make the model less numerically demanding.

We already assumed that all cells are of the same size and all have the same internal volume. Next let us assume that all cells have the same initial soluble coffee mass, i.e. all cells have the same initial coffee mass concentration.

As with many numerical techniques, we discretise the solution domain (the puck) into a set of S thin horizontal strips (here we assume that the water moves from the top to the bottom of the puck, as in an espresso machine). The coffee concentration within a strip is assumed to be constant, and it needs just one variable $m_{between,\ s}$ to track the soluble coffee mass between the grains in a strip number s.

Next let us turn to spherical grains which are built from concentric cell layers (see Figure 1). As the initial coffee concentration within cells is the same for all cells, and the coffee concentration is constant within the puck strip, then it is enough to have one variable per cell layer to track the mass for all cells within this layer. E.g. for all grains with 3 cell layers in a given puck strip we need only 3 variables to track the coffee mass. Note that for all grains with e.g. 4 cell layers we need another 4 variables, as the diffusion dynamics is different for cells with 3 and 4 layers.

So the idea to discretise the puck into strips and consider cell layers within a coffee grain which all follow the same diffusion dynamics reduces the number of variables considerably and makes the numerical implementation not so challenging.

In the software we introduce a matrix with 3 indexes: s (the puck strip number), g (the grain size index) and n (the cell layer number within the grain) – to track the soluble mass within cells. Then we use a set of rules to update the mass values within the matrix. This is why we call this approach the mass transfer matrix espresso extraction model.

Rules for the mass matrix update

We need to make some changes to Equation 3 and 4, to account for the number of cells within each cell layer.

This is how we calculate the number of cells per each layer. We calculate a single cell volume using the formula for a sphere:

$$V_{cell}^{total} = \pi \cdot \frac{{D_{cell}}^3}{6} \quad (5)$$

Here Dcell is

Number of cell layers	Grain diameter. mm	Grain volume, mm3	Number of cells per grain	Number of cells in the top layer
1	0.03	1.41372E-05	1	1
2	0.09	0.000381704	27	26
3	0.15	0.001767146	125	98
4	0.21	0.004849048	343	218
5	0.27	0.010305995	729	386

Table 1. Calculations of the number of cells per grain and per cell layer.

Table 2 lists the variables used and their typical values, as per [1] and [2]. The formulae used to calculate the values are given after the table.

Description	Value	Name in the software	Notation in equations
Basket / puck diameter, mm	58.5	puck_diameter_mm	D_{puck}
Coffee cell diameter, mm	0.03	coffee_cell_diameter_mm	D_{cell}
Bean weight, g	18	dsv2_bean_weight	M_{bean}
Top of the puck area, mm^2	2688		
Puck volume, mm^3	54546		
Puck height, mm	20.29		

Table 2. List of variables and their typical values, as per [1] and [2].

$$K^* = K \cdot V_{cell} \quad (2)$$