

THE ESPRESSO COFFEE PROBLEM

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1 Introduction

Espresso coffee - consumed millions of times a day around the globe - is on closer inspection of high complexity. It is not without reason that many Italians consider the preparation of a perfect espresso as high art and enter into a relationship of trust with their favourite barista. Scientifically speaking, the preparation of a cup of espresso is a fluid process that takes place at high temperatures and pressure.

The task was kept open to cope with the high complexity of the problem and to allow creative modelling approaches. First the goal and some basics of coffee will be described. In the main part the process of flowing through the espresso powder is divided into the sub-aspects of mechanics and chemistry for modelling. It was found that the bimodality of the size distribution of ground coffee beans significantly influences both sub-problems. As described in the third chapter of the report, in the mechanical modelling, the espresso powder presents a flow resistance that is highly nonlinear due to the different particle sizes. This behaviour could be mapped using differential equations in the mechanics model. In the chemical model, which depicts the solution process of the coffee powder, the different particle sizes act as source terms with very different time constants. Details are discussed in the fourth chapter of the report. The merging of the submodels allows trend forecasts for the adjustment of process parameters to ensure the preparation of a perfect espresso and is still to be further investigated as is stated in chapters 5 and 6. In Chapter 7 we will take a look at the group work dynamics before the report is closed in chapter 8 with the instructor's assessment.

2 Project "Espresso Coffee Problem"

Before the actual modelling of the "Espresso Coffee Problem" is discussed we will present the goal of the project, data that was used during the modelling and our approach to start the modelling with in this chapter.

2.1 Goal of this project

Due to the short amount of time given, we decided to focus on two single aspects of the whole extremely complex problem of coffee preparation, namely:

- The mechanical modelling of a flow passing through the cake of grounded coffee powder,
- the modelling of the solution process of soluble coffee substances into the water flowing through the cake.

While the chemistry of the solution process is dependent on the mechanics of the flow the development of the two models was started with low dependency due to the short amount of time and the low number of scientists available. The goal was to have a basic model for each aspect so in a next step it could be further investigated how to combine those into a fully descriptive "Espresso Coffee Model".

2.2 Objective and data available

In figure 1 is shown a simplified model of the preparation of espresso coffee.

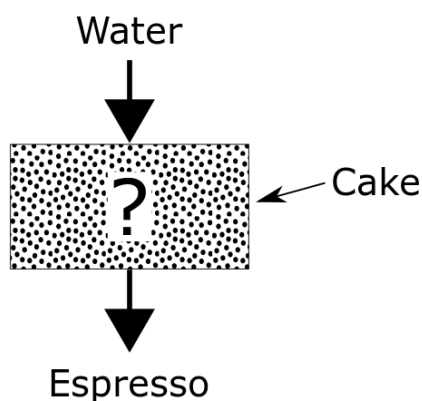


Figure 1: Simplified model of coffee preparation

For the modelling of the preparation the focus was on the mechanisms that act inside the so called coffee cake. All auxiliaries inside the coffee machine are neglected and it is assumed that hot water is pushed through a container densely packed with grounded coffee to get an outflow of coffee.

As a first step to mechanical modelling the system described above can be seen as a fluid-mechanical problem. The water is an inflow while the coffee is an outflow. Applying the Bernoulli's law neglecting gravity we get:

$$(p_{in} + \rho \frac{u_{in}^2}{2}) - (p_{out} + \rho \frac{u_{out}^2}{2}) = -R. \quad (1)$$

The change in total pressure $(p + \rho u^2/2)$ between inlet and outlet is due to a hydraulic resistance (R) in the coffee cake. How this resistance is dependent on boundary conditions and how it can be modelled is explained in chapter 3.

2.3 Size Distribution of Grounded Coffee

The following section will give a short introduction in the bimodality of the size distribution of grounded coffee since this is of high importance for both the mechanical model discussed in chapter 3 as well as the chemistry model discussed in chapter 4.

As can be seen from experimental investigations grounded coffee contains particles of different sizes. Particle sizes are influenced by the type of coffee beans that are used and also on the grounding process. Nevertheless size distributions have a bimodal shape. There is a peak in the volume fraction around $25 \mu m$ and a higher peak around $300 \mu m$ as can be seen from figure 2.

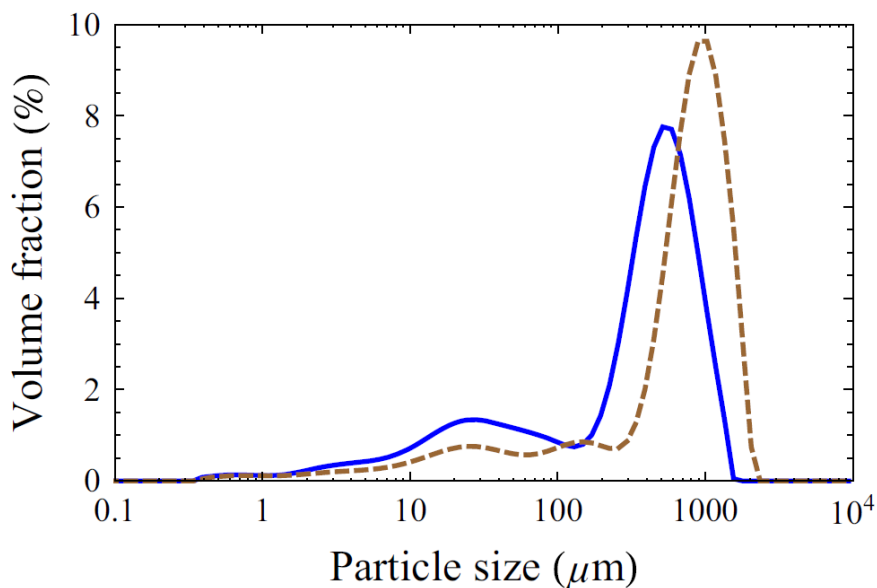


Figure 2: Representative particle size distributions (taken from Moroney et al. (2015))

Dealing with a continuous function for the size distribution is of high complexity for modelling. For this reason the size distribution function was approximated by two representative particles - namely a small and a big particle. It is assumed that those two representative particles are able to capture the mean macroscopic behaviour of the original continuous distributed particles.

To extract the identifying particles, in a first step the experimental data is fitted to a continuous function. We use the sum of two Gaussian functions to reconstruct the bimodal appearance of the particle size distribution:

$$\nu(d) = \frac{1}{\sigma_1\sqrt{2\pi}} \exp^{-\frac{1}{2}\left(\frac{d-\mu_1}{\sigma_1}\right)^2} + \frac{1}{\sigma_2\sqrt{2\pi}} \exp^{-\frac{1}{2}\left(\frac{d-\mu_2}{\sigma_2}\right)^2}. \quad (2)$$

Now this function can be used to get the representative particle sizes and their volume fractions. We transform the continuous function into two Diract- δ -peak-functions.

Therefore a threshold-size is defined and the mean weighted radii are calculated:

$$\bar{r}_{small} = \int_0^{r_T} r_i \nu_i d\tilde{r}, \quad (3)$$

$$\bar{r}_{big} = \int_{r_T}^{\infty} r_i \nu_i d\tilde{r}. \quad (4)$$

To these mean radii we can then match the belonging volume fraction:

$$\nu_{small} = \frac{\int_0^{r_T} \nu_i d\tilde{r}}{\int_0^{\infty} \nu_i d\tilde{r}} \quad (5)$$

by dividing the volume of small particles by the total volume. With that we easily get ν_{big} by:

$$\nu_{big} = 1 - \nu_{small}. \quad (6)$$

Using this transformation procedure we now have access to two distinct representative particles we know size and volume fraction of.

In figure 3 the size distribution of the particles is shown and the dimension of the small and the big particles is highlighted. It can be seen that the size of the big particles is roughly 10 times the size of the small ones.

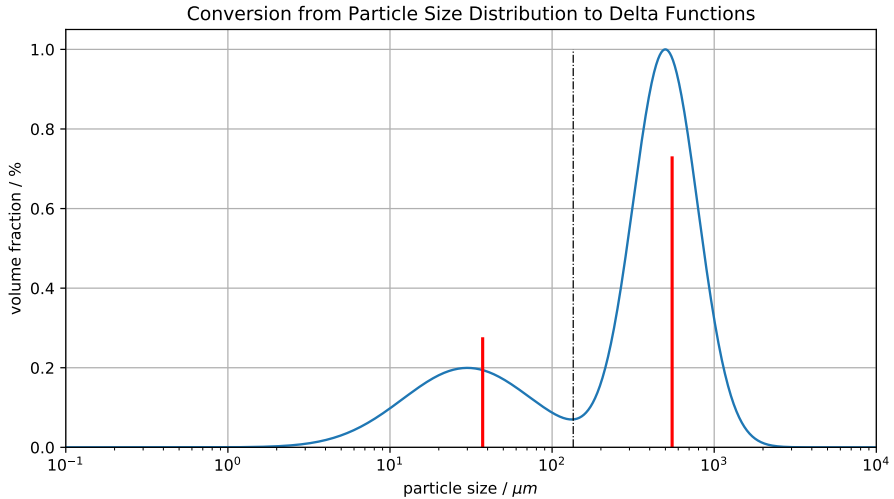


Figure 3: Approximate particle size distribution is shown in blue, with the size and volume fraction of big and small particles highlighted in red.

3 Particle Sizes influencing Mechanics

3.1 The compact layer

The presence of particles of different sizes, explained in the previous section, influences the mechanical behaviour of the production of coffee.

Figure 4 shows the microscopical structure of the coffee cake. At the initial time, before the water goes through the coffee cake, the small particles are uniformly distributed in the container and some of them are bounded to the big particles, because of the oily substances present in the system and possibly also for bonds of electric type.

When the process starts and the water enters the containers, the flow breaks some of the bonds and transport some of the the small particles, which reach the end of the container that is permeable to liquid, but not to the solid component. As a result, the fine particles will build up a layer at the end of the container, called the compact layer, which has a resistance much larger than the rest of the container.

As time increases and the removal process goes on, the resistance in the compact layer is assumed to be constant, but the thickness of the compact layer grows, resulting in a rise of the total resistance in the container. The thickness of the compact layer reaches then an asymptotic value, called S_{max} , and so does the total resistance.

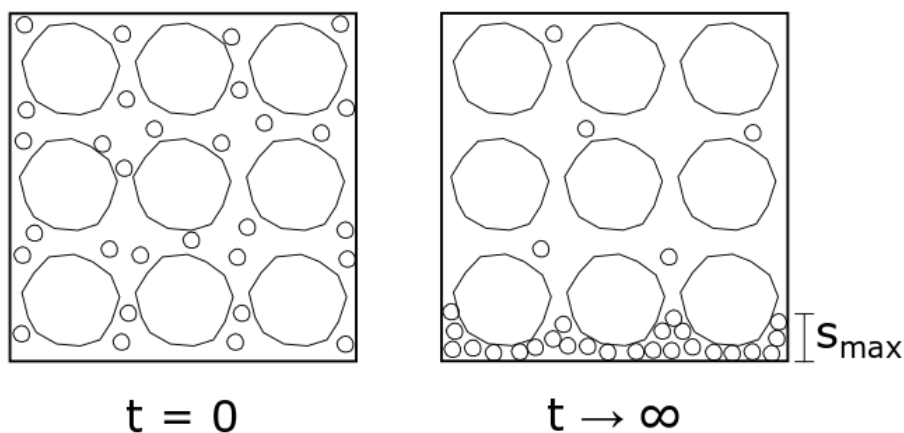


Figure 4: Microscopical structure of the coffee cake. A detailed description of this figure is given in the text.

Let us now model analytically the behaviour of the compact layer.

We assume that the process is described by a one-dimensional model because the physical problem suggests that filtration can be considered in a good approximation predominant in the axial direction. We therefore introduce the x -axis which is directed from the top to the bottom of the coffee cake. Thus in our model, the upper layer of the container is located at $x = 0$ and the bottom layer of the coffee cake is located at $x = L$, where L denotes the length of the container.

The x -coordinate of the upper bound of the compact layer changes in time and is denoted by $s(t)$. Therefore the region with $0 < x < s(t)$ represents the upper layer of

the container, while the part with $s(t) < x < L$ is the compact layer.

At the initial time $t = 0$, the fine particles are not compacted yet and the thickness of the compact layer is zero. Thus the initial condition is $s(0) = L$.

When the water goes through the coffee grains, the compact layer starts growing until it stabilises, reaching its asymptotic thickness S_{max} . Therefore the coordinate $s(t)$ decreases in time, until it reaches its asymptotic value $L - S_{max}$.

Since the pressure of the water moves the compact layer border very rapidly, a reasonable choice to describe the position $s(t)$ of the upper border of the compact layer with respect to time is a decreasing exponential function.

The formula we have used for the coordinate $s(t)$ is the following:

$$s(t) = L - S_{max}(1 - e^{-Ct}), \quad (7)$$

where C is a constant to be determined.

The following figure represents exactly how the compact layer behaves.

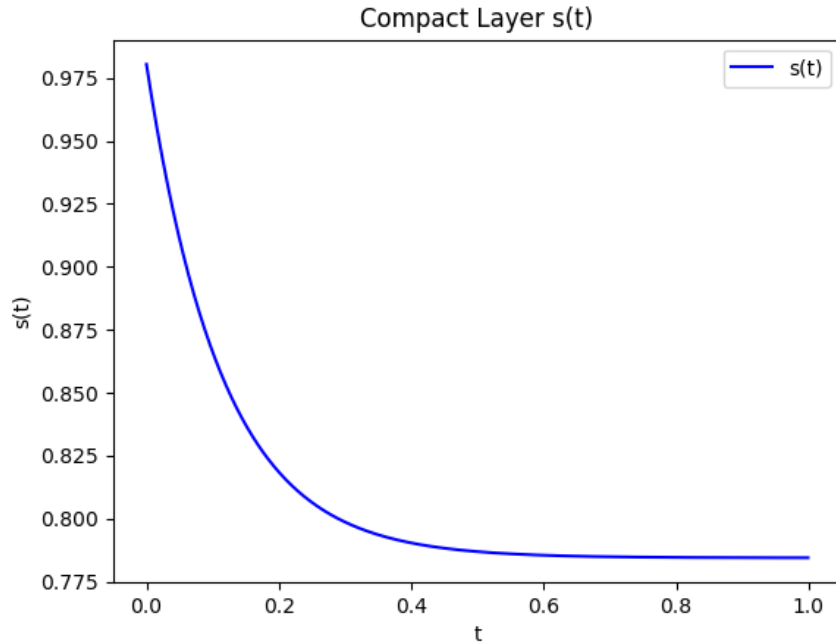


Figure 5: Illustration of the behaviour of the compact layer.

3.2 Experimental Discharge

The experimental approach is a naive approximation of coffee preparation. To obtain the ideal cup of coffee, the temperature and pressure need to be correctly adjusted. In order to provide an approximation of the model, Darcy's law is used and gives the following equation,

$$p = Rq \quad (8)$$

where p is the injection pressure, q the volumetric velocity and R the hydraulic resistance of the cake.

However, experimental observations prove a contradiction to Darcy's law, since

- flow has not a linear behaviour as it attains a sharp maximum in the beginning of the procedure and then reaches an asymptotic value,
- there is no proportionality of the asymptotic value and the pressure.

These observations are visualised by the figure [6]. Temperature dependence of the model influence this non-linear effect. Even, by injecting low temperature water this non-monotone effect is occurred. The following part is dedicated to the manipulation of experimental data in order to approximately implement the discharge and remark the observations mentioned above.

The discharge q is approximately expressed as a function of time as follows,

$$q(t) = a + de^{-ct}, \quad (9)$$

where

- a expresses the value of discharge when time tends to infinity,
- d is the difference between a and the maximum of the curve,
- c is chosen as $1 - \frac{1}{\Delta p}$, where Δp signifies the difference between the initial and the final pressure.

In order to have explicit values of the previous coefficients, a graph of the article Fasano, Talamucci, and Petracco (2000) is used. The following table represents their values for different gradient pressures.

Δp	a	d
3	0	14
5	5	16
7	4	13

Table 1: Discharge coefficients for different Δp .

As the number of given points is small, we did an interpolation for a and d given by,

$$\begin{cases} a(\Delta p) = -\frac{3}{4}\Delta p^2 + \frac{17}{2}\Delta p - \frac{75}{4} & (10) \\ d(\Delta p) = -\frac{5}{2}\Delta p^2 + 6\Delta p + \frac{13}{8} & (11) \end{cases}$$

The following figure illustrates the discharge as a function of time for different values of Δp . The initial pressure is $p_0 = 8$ bars.

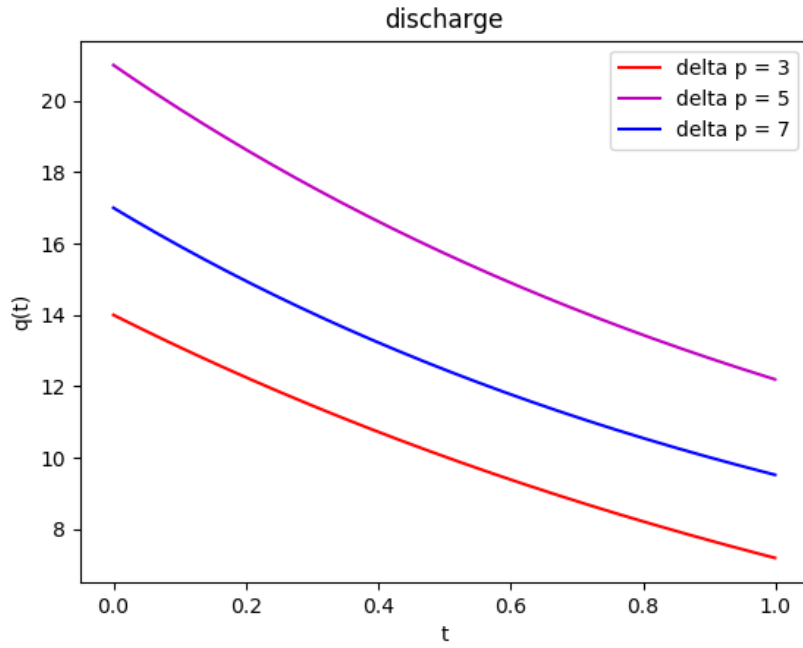


Figure 6: Plot of the experimental discharge as a function of time for $\Delta p = 3, 5, 7$.

3.3 Modelling the problem

We can now start modelling the problem. Let us call b the concentration (i.e. mass per unit volume of the total system) of the fine particles when they are bounded to the big particles and m the concentration of the small particles that are transported by the flow. Our goal is to find some equations to describe the behaviour of b and m with respect to time and space.

3.3.1 Stable Particles

Let's start setting a model for b . We assume that during the particle removal process, not all the fine particles can be removed, but only those ones with bonds that are weak enough. Such a behaviour is modelled by introducing a threshold function $\beta(q)$ such that the particle removal process occurs only as long as the concentration b exceeds the value of $\beta(q)$.

We suppose that $\beta(q)$ is a decreasing function of q , because the more intense a flow is, the larger the amount of removable fine particles is. The effect of the threshold is that, since typically q decreases in time, β will increase and may switch off the removal process at some time.

As stated in Fasano, Talamucci, and Petracco (2000), the production rate of stable particles in the upper layer of the coffee cake is described by the following equation:

$$\begin{cases} \frac{\partial b}{\partial t} = -q(t)[b - \beta(q)]^+, & 0 < x < s(t), \quad t > 0, \\ b(0) = b_0 > 0, \end{cases} \quad (12)$$

where the symbol $[\cdot]^+$ denotes the positive part and b_0 is the concentration of bounded fine particles at the initial time $t = 0$.

Equation (12) models the fact that if $b > \beta$, the production rate is proportional to the discharge q while if $b < \beta$, the concentration b is constant in time which means that no more fine particles are removed and therefore the removal process has stopped.

An important feature of the concentration b is that it is constant with respect to x and thus equation (12) becomes:

$$\begin{cases} \frac{db}{dt} = -q(t)[b - \beta(q)]^+, & t > 0, \\ b(0) = b_0 > 0. \end{cases} \quad (13)$$

This is a consequence of having chosen a constant value for b at $t = 0$ and of q depending only on t . It can be proofed using equation (12) in the following way: if $b > \beta(q)$,

equation (12) becomes

$$\frac{\partial b}{\partial t} = -q(t)(b - \beta(q(t))),$$

from which we get

$$\frac{\partial b}{\partial t} + q(t)(b - \beta(q(t))) = 0. \quad (14)$$

Then, taking the derivative of (14) with respect to x we get

$$\frac{\partial}{\partial x} \left(\frac{\partial b}{\partial t} + q(t)(b - \beta(q(t))) \right) = 0$$

and thus

$$b_{tx} + q(t)b_x = 0. \quad (15)$$

From (15), we read that $b_t + q(t)b$ doesn't depend on x , but it's only a function of time t and therefore $b = b(t)$. We have now proved that b is constant with respect to x when $b > \beta(q)$.

Let us now consider the case $b \leq \beta(q)$. In this case equation (12) becomes

$$\frac{\partial b}{\partial t} = 0,$$

and this b is constant through time. Since we have chosen a constant value b_0 for b at $t = 0$, then b doesn't depend on x in this case either.

Let us now numerically solve Equation (13) with respect to b , for values of time $t \in [0, 1]$ and with initial value given by $b_0 = 1$. In regards to $q(t)$, we have inserted into Equation (13) the expression of the experimental discharge $q(t) = a + de^{-ct}$ with values of the constants a, d, c derived in the previous section. For the threshold $\beta(t)$, we have chosen the following decreasing function of $q(t)$:

$$\beta(q(t)) = q(0) - q(t),$$

where $q(t)$ is given by the experimental discharge. The constant $q(0)$ is chosen so that at time $t = 0$ the threshold function β is zero and therefore the removal process starts certainly at $t = 0$.

In order to numerically solve Equation (13), we first solve the corresponding equation without the positive part, given by

$$\begin{cases} \frac{d\bar{b}}{dt} = -q(t)[\bar{b} - \beta(q)], & t > 0, \\ \bar{b}(0) = b_0 > 0, \end{cases} \quad (16)$$

with respect to \bar{b} , using a finite difference scheme.

The resulting finite difference scheme is given by:

$$\bar{b}(t_{i+1}) = \bar{b}(t_i) - \Delta t \left(a + de^{-ct_i} \right) \left(\bar{b}(t_i) - d + de^{-ct_i} \right) \quad i = 1, \dots, N - 1$$

where we have divided the interval $[0, 1]$ in $N = 1000$ equally spaced points

$$t_0 = 0, t_1, \dots, t_{N-1}, t_N = 1$$

and we denote $\Delta t = t_{i+1} - t_i \quad \forall i$.

Once we have the numerical solution for \bar{b} , we recover the approximate solution b of Equation (13) by cutting the function \bar{b} at its global minimum and, from that point on, using a constant value for b , chosen in order to preserve the continuity of the function. The cutting point represents the time in which β becomes large enough to stop the removal process.

The resulting numerical solution for $b(t)$ is shown in Figure 7. We can see that $b(t)$ decreases very fast in time and reaches quickly its asymptotic constant value. This means that the removal process happens really fast and it stops in a short time.

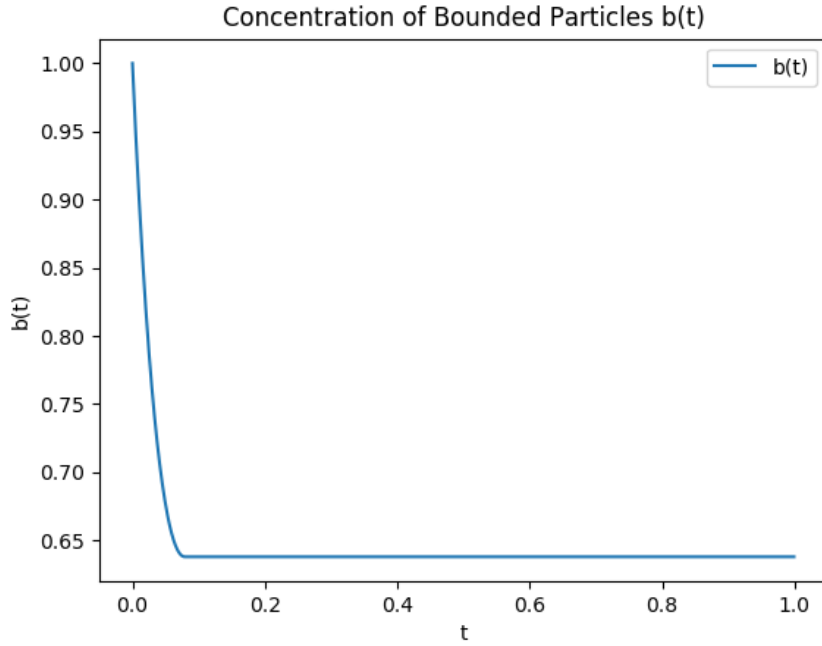


Figure 7: Plot of the numerical solution of Equation (13) with respect to b , with $t \in [0, 1]$, $b_0 = 1$, $q(t) = a + de^{-ct}$, $\beta(q(t)) = q(0) - q(t)$.

3.3.2 Moving Particles

After modelling the stable particle concentration, we proceed to the fine particles that are free to move. In order to find the formula of the moving particles, the characteristics method is used.

First let us introduce the differential equation of the production rate of moving particles as stated in Fasano, Talamucci, and Petracco (2000),

$$\begin{cases} \frac{\partial m}{\partial t} + \mu q(t) \frac{\partial m}{\partial x} = -\frac{db}{dt}, & \text{for } 0 < x < s(t), t > 0, \\ m(x, 0) = m_0(x) > 0, & \text{for } 0 < x < s(t), \\ m(0, t) = 0, & \text{for } t > 0. \end{cases}$$

The characteristics method is applied on the sum of b and m and then m is easily found as we already know b from the previous section. This can be accomplished as b is independent of space, which means $\frac{\partial b}{\partial x} = 0$.

Using this assumption, the differential equation of the moving particles is transformed as,

$$\frac{\partial(m+b)}{\partial t} + \mu q(t) \frac{\partial(m+b)}{\partial x} = 0$$

By imposing $u = m + b$, the problem we search to solve is transformed to a transport differential equation,

$$\begin{cases} \frac{\partial u}{\partial t} + \mu q(t) \frac{\partial u}{\partial x} = 0, \\ u(x, 0) = m_0(x) + b_0. \end{cases}$$

First, we need to solve the following system in order to find the characteristic curve related to (x, t) . This system is composed by the differential equation equal to the coefficient of the partial derivative of u with respect to the space and the position of the characteristic curve at a given time t .

Let (x, t) fixed.

$$\begin{cases} X'(s) = \mu q(s) & \text{for } s > 0, \\ X(t) = x \end{cases} \quad (17)$$

The solution of the previous system is devoted by $X(s)$ and is called characteristic curve.

The solution, after imposing the experimental discharge $q(t) = a + de^{-ct}$, is given by,

$$X(s) = \mu(a(s-t) + \frac{d}{c}(e^{-ct} - e^{-cs})) + x$$

Along the characteristic line, for example for $s = 0$, the solution to the differential problem remains constant.

In order to complete the characteristics method and find the solution to the problem, the following equation needs to be solved.

$$\begin{cases} Z'(s) = 0 \\ Z(0) = u(X(0), 0) = m_0(x + \mu(-at + \frac{d}{c}(e^{-ct} - 1))) + b_0 \end{cases} \quad (18)$$

The solution of the previous system is

$$Z(s) = m_0(x + \mu(-at + \frac{d}{c}(e^{-ct} - 1))) + b_0 \quad (19)$$

The characteristics method provides the solution when the variable of Z is the time across the characteristic line, $u(X(t), t) = Z(t)$. Finally, the solution for u is,

$$u(x, t) = (m + b)(x, t) = m_0(x + \mu(-at + \frac{d}{c}(e^{-ct} - 1))) + b_0 \quad (20)$$

As the b was previously solved, the m formula can be easily deduced.

Figure 8 represents the behaviour of m as a function of time for $x_0 = 0.1$ and initial condition $m_0(x) = e^{-x^2}$.

From the plot, we can see that, as the water goes through the coffee, some of the particles start to move. After reaching a sharp maximum, the concentration of moving particles starts decreasing as the compact layer increases radically.

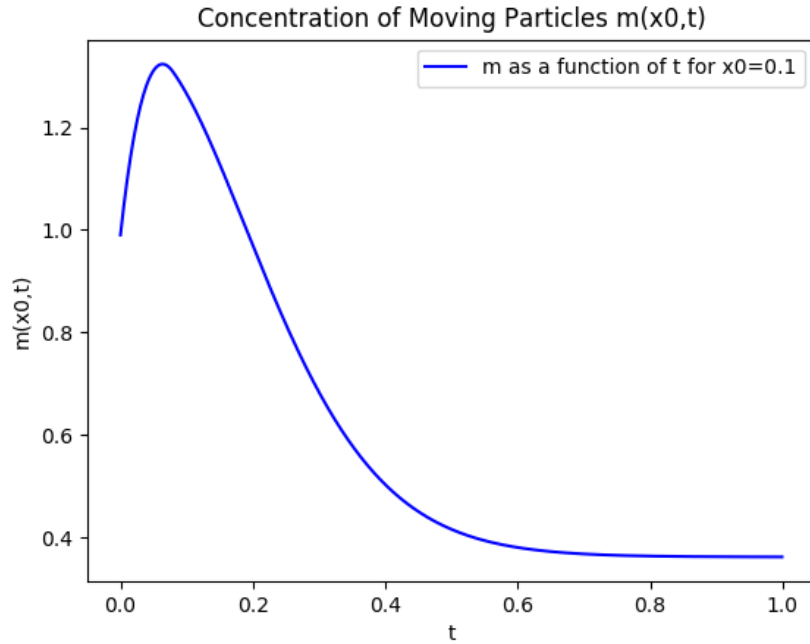


Figure 8: Plot of the concentration of moving particles m as a function of time for $x_0 = 0.1$ and initial condition $m_0(x) = e^{-x^2}$.

3.3.3 Discharge

After having set up a model for the concentrations b and m , we are now interested in modelling the discharge $q(t)$. We can then write Darcy's law above and below the boundary of the compact layer:

$$\begin{aligned} q(t) &= -K_1(b, m) \frac{\partial p}{\partial x}, & 0 < x < s(t), & \quad t > 0, \\ q(t) &= -K_2 \frac{\partial p}{\partial x}, & s(t) < x < L, & \quad t > 0, \end{aligned} \tag{21}$$

where $\frac{\partial p}{\partial x}$ signifies the pressure gradient of the two parts of the container, K_1 is the hydraulic resistance above the compact layer boundary and K_2 is the hydraulic resistance of the compact layer.

It is important to mention that the hydraulic resistance of the compact layer is significantly higher than the other one.

Now, we have a complete mechanical model for the espresso coffee problem, given by:

$$\begin{cases} \frac{\partial m}{\partial t} + \mu q(t) \frac{\partial m}{\partial x} = -\frac{db}{dt}, & 0 < x < s(t), t > 0, \\ \frac{db}{dt} = -q(t)[b - \beta(q)]^+, & t > 0, \\ q = -K_1(b, m) \frac{\partial p}{\partial x}, & 0 < x < s(t), t > 0, \\ q = -K_2 \frac{\partial p}{\partial x}, & s(t) < x < L, t > 0, \end{cases}$$

with the following initial conditions,

$$\begin{cases} b(0) = b_0 = 1, & 0 < x < L, \\ m(x, 0) = m_0, & t > 0, \\ m(0, t) = 0, & \\ s(0) = L, & \\ p(0, t) = p_0, & t > 0, \\ p(L, t) = 0 & t > 0. \end{cases}$$

We are now interested in finding a unique explicit formula for the discharge $q(t)$; for this purpose, the fundamental theorem of calculus is used:

$$\int_0^L \frac{\partial p}{\partial x} dx = p(L) - p(0) = -p_0. \tag{22}$$

Then, using (21), we get:

$$\begin{aligned}
\int_0^L \frac{\partial p}{\partial x} dx &= \int_0^{s(t)} \frac{\partial p}{\partial x} dx + \int_{s(t)}^L \frac{\partial p}{\partial x} dx \\
&= \int_0^{s(t)} -R_1(b, m)q(t) dx + \int_{s(t)}^L -R_2 q(t) dx \\
&= -q(t) \left(\int_0^{s(t)} R_1(b, m) dx + R_2(L - s(t)) \right),
\end{aligned} \tag{23}$$

where we introduced the resistivity in the two layers $R_1(b, m) = \frac{1}{K_1(b, m)}$ and $R_2 = \frac{1}{K_2}$. Therefore, from (22) and (23) we get

$$q(t) = \frac{p_0}{\int_0^{s(t)} R_1(b, m) dx + R_2(L - s(t))} \tag{24}$$

where p_0 is the pressure difference between the upper and the bottom layer of the container.

In figure 9, we show the behaviour of the theoretical discharge obtained using the formula (24), with the following values of the parameters: $L = 1$ and $p_0 = 8$. Regarding the choice of the x -coordinate of the upper bound of the compact layer $s(t)$, we have used, according to (7), the following formula:

$$s(t) = 1 - 0.2(1 - e^{-0.8t}). \tag{25}$$

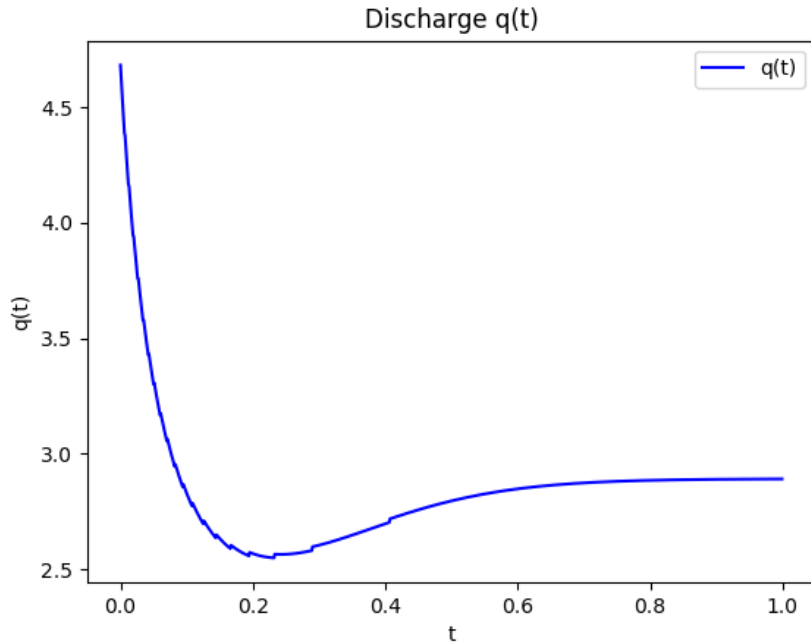


Figure 9: Illustration of the theoretical discharge given by (24) with $L = 1$, $p_0 = 8$ and $s(t) = 1 - 0.2(1 - e^{-0.8t})$.

It is remarkable to notice that the graphs of the experimental and theoretical discharge are quite similar.

It is important to mention the choice we have done for the resistivity in the two layers, in order to provide an implementation of the problem. The resistivity above the compact layer we used is defined as a linear combination of b and m :

$$R_1(x, t) = b(t) + m(x, t).$$

As mentioned before, the resistivity of the compact layer is importantly higher than the one above the layer and constant. That is the reason why it is chosen as

$$R_2 = 10 \cdot R_1(x_0, t_0),$$

where x_0, t_0 are arbitrary.

Finally, figure 10 represents the behaviour of R_1 as a function of time, for a given $x_0 = 0.4$.

It worth highlighting that we initially had some difficulties in finding a function that modelled properly the resistivity $R_1(x, t)$, namely a function that had the expected behaviour with respect to time and space. This problem was finally overcome by the choice of the function $R_1(x, t) = b(t) + m(x, t)$, using $m_0(x) = e^{-x^2}$ as initial condition for $m(x, t)$ at $t = 0$.

From figure 10 we can see that the resistivity above the compact layer grows in the first time interval, when the concentration of moving particles is increasing, and then when m starts decreasing, so the resistivity does. This is the behaviour that we expect for the resistivity above the compact layer, with respect to time.

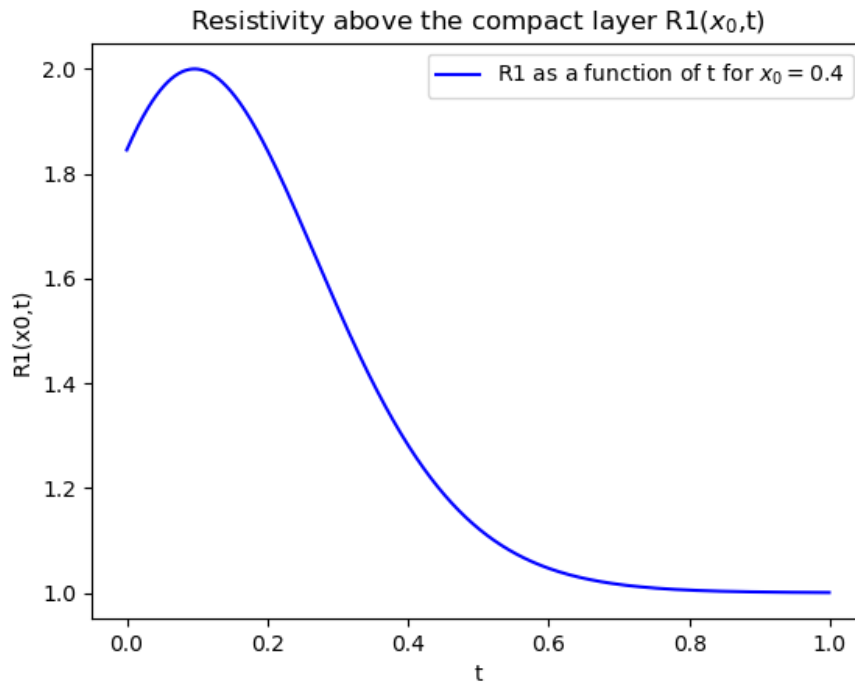


Figure 10: Plot of the resistivity above the compact layer as a function of time t , for $x_0 = 0.4$.

4 Modelling of Coffee Chemistry

The mechanical modelling is based on observations at conditions where solution processes can be neglected. Anyhow an espresso is not just hot water but there are several chemical substances solved in. In this chapter we focus on modelling the processes that lead to the solution of substances into the hot water flowing through the coffee cake.

One basic assumption of the moving boundary theory is that the coffee cake is already completely saturated. This ignores the initial transient process of a moving waterfront propagating through the coffee cake. The final state of the imbibition process is used as an initial state for the formation of the separated layers. While this assumption is justified for the modelling of the layers it is not with respect to the chemical processes. As can be told from the very basic experiment of preparing a coffee the initial phase is crucial - at first the coffee comes out strongly black and then becomes lighter with time. The colour is an indicator for the amount of coffee molecules solved in the water. This means that initially there is a high rate of solution which is decreasing in time.

Having figured out the importance of the initial phase it is obvious that for the modelling we have to focus on a different part of the preparation time than we did for the mechanical aspects.

Before starting the description of modelling it is essential to take a look at the structure of coffee particles. As mentioned before we consider the properties of grounded coffee to be described by only two different particle sizes. There are small particles with a peak around $\bar{r}_{small} \approx 40 \mu m$ and big particles having a peak at $\bar{r}_{big} \approx 550 \mu m$. Those behave different with regards to solution due to the average size of a coffee cell being around $25 - 50 \mu m$. This means that small particles to a high amount are considered as cell fragment or broken cells while the big particles consist of an agglomerate of intact and broken cells as is sketched in figure 11.

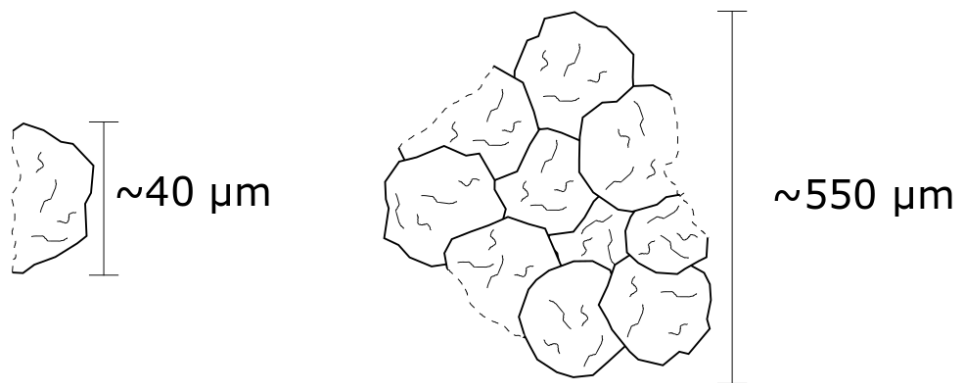


Figure 11: Structure of particles: Broken cell walls are shown as dashed lines

While coffee is a rather complex substance composed of over 1800 chemical compounds (compare Petracco (2008)) we consider coffee to only consist of two entities which are soluble and insoluble substances. Those soluble compounds are sketched in figure 11 as

exemplary molecules inside the cell. Due to the high temperature of around 900° C it is assumed that solution processes are very quick. Once a soluble substance gets in contact with water it is considered to be solved instantaneously. Experimental observations by Dentan (1977) showed that extraction mainly appears on the outer surface because soluble substances are well protected inside the cell. With the protecting cell wall around them broken, in small particles those substances are easily accessible for a surrounding flow. This allows for convective transport to happen taking the soluble substances out of the cell. The timescale of this extraction is very small. Convection is fast and starting nearly without dead time making it the dominant process at the initial phase of the preparation.

Big particles also contain broken cells that distribute to the total amount of solved coffee with the same mechanism as the small particles. But in addition they also consist of intact cells. The soluble substances in those are well protected by the cell walls so the dominant mechanism of transporting them to the surface of the cell where they will be picked up by convection is diffusion. Diffusion in general has a much larger timescale than convection making it a slower process. Adding to that, diffusion is forced by a gradient of concentration which will decrease over time. Those two observations justify the assumption that diffusion will start to contribute to the overall solution of coffee molecules at a later point.

4.1 Initial Phase

The explanations of the previous section are used to develop a model allowing to estimate the mass of soluble substances that were solved in the coffee during an initial phase. Modelling the real processes would be rather complex so we use an integral method. We look at the time $t = T_{init}$ when we consider the initial convective transport to have solved most of the soluble substances accessible by broken cell walls and having discharged them out of the coffee container. This allows us to model the complex processes happening for $0 \leq t \leq T_{init}$ by approximating the final state at $t = T_{init}$ as the result of those processes. Within the next sections we will model the mass of extracted coffee by making use of information about the size distribution within the grounded coffee.

4.1.1 Small Particles

We know the volume fraction of small particles ν_{small} so with the total mass of coffee m_{coffee} we know the mass of small particles assuming that the density of coffee is similar for both,

$$m_{small} = \nu_{small} \cdot m_{coffee}. \quad (26)$$

To compute the mass of solved substances $\zeta_{small} \leq 1$ and $\gamma_{small} \leq 1$ are introduced. While ζ_{small} is the fraction of mass that is soluble, γ_{small} is used to take in account that

not all smart particles might have been affected by the initial solution process. With that we get the solved mass coming from the small particles in the initial phase as:

$$m_{small,solved} = m_{small} \cdot \zeta_{small} \cdot \gamma_{small}. \quad (27)$$

4.1.2 Big Particles

For the big particles' contribution to the solved mass of coffee we need to adapt the modelling. This is due to the consideration that only the broken cells on the surface are contributing to the initial solution. First we compute the total surface of big particles. The volume of big particles is defined by:

$$V_{big} = \nu_{big} \cdot \frac{m_{coffee}}{\rho_{coffee}}. \quad (28)$$

We assume all particles to be of spherical shape. This allows us to make use of the surface to volume fraction $\psi = \frac{3}{r}$. We then get the surface as follows:

$$S_{big} = V_{big} \cdot \frac{3}{\bar{r}_{big}}. \quad (29)$$

For estimating the volume addressed by the convection we assume the height of the active surface to be equal to the size of the small particles. We also introduce $\xi_{big} \leq 1$ which takes into account the fraction of broken cell walls on the surface compared to the total surface,

$$V_{big,active} = S_{big} \cdot \bar{r}_{small} \cdot \xi_{big}. \quad (30)$$

Again we have ζ and γ as before and get the solved coffee mass coming from the big particles in the initial phase as:

$$m_{big,solved} = V_{big,active} \cdot \rho_{coffee} \cdot \zeta_{big} \cdot \gamma_{big}. \quad (31)$$

The amount of solved substances discharged at time $t = T_{init}$ is computed by summing up the solved masses coming from both the small and the large particles. In addition the fraction of solved mass can be computed,

$$m_{solved}(t = T_{init}) = m_{small,solved} + m_{big,solved}, \quad (32)$$

$$\chi(t = T_{init}) = \frac{m_{solved}(t=T_{init})}{m_{coffee}}. \quad (33)$$

4.2 Subsequent Phase

After the initial time where there is instantaneous solution as a dominant process with increasing time diffusion becomes more important. While we considered our flow to be one-dimensional, diffusion always is multidimensional. This and the coupling of flow, convection and diffusion would lead to a complex problem to solve. Instead of dealing with that we therefore propose a basic model based on an exponential function.

The results of the initial phase modelling are used as an initial boundary condition of this modelling. With $t^* = t - T_{init}$ the initial extracted mass fraction is $\chi(t^* = 0) = \chi(t = T_{init})$. From literature we get an upper bound for the maximum mass fraction that is extractable from coffee as ζ_{coffee} . We then express the extracted mass fraction over time by:

$$\chi(t^*) = \zeta_{coffee} \cdot \left(1 - \left(1 - \frac{\chi(0)}{\zeta_{coffee}} \right) \cdot \exp\left(-\frac{t^*}{\tau}\right) \right). \quad (34)$$

With this approach the only unknown is τ which can be tuned when experimental data is available.

The modelling of χ using an exponential function is justified considering the underlying processes. The initial instantaneous solution processes are fading out with the solved substances discharged. With that the concentration changes and diffusion become more dominant. Diffusion is happening on a large timescale making it a relative slow process which also affects the solution. As time continues the gradient of concentration becomes smaller because the amount of soluble substances inside the intact cells is decreasing. Being the main force of diffusion processes the diffusion will also slow further down over time. Summing this up, the rate of solution is monotonously decreasing while χ is monotonously increasing. The knowledge of an upper limit for ζ_{coffee} that is reached after a long extraction time and cannot be further increased by heighten the extraction time fits well with the asymptotic behaviour of an exponential function. The free constant τ is considered to be dependent on the temperature of the process, the grinding process of the coffee beans that affects the size distribution of particles, the pressure difference and finally the coffee machine's geometry which affects the raise of the pressure, the flow's velocity by defining the flowed through area and the efficiency of the solution process in general.

5 Application of chemistry model

The proposed model of chemistry introduced in the previous section will be applied to a concrete set of values explained in the following.

5.1 Initial Phase

We assume the amount of grounded coffee used for preparation to be $m_{coffee} = 10 \text{ g}$ and its density $\rho_{coffee} = 400 \text{ kg/m}^3$. The fraction of extractable soluble substances in grounded coffee is set to $\zeta_{coffee} = 0.3$ following Moroney et al. (2015). We get mean size and volume fraction of the particles as mentioned before as $\bar{r}_{small} = 40 \mu\text{m}$, $\bar{r}_{big} = 550 \mu\text{m}$, $\nu_{small} = 0.25$, $\nu_{big} = 0.75$. We choose $\zeta_{small} = 0.25$ and $\zeta_{big} = 0.25$ assuming that the amount of soluble substances addressable by instantaneous solution is around 80 % of ζ_{coffee} . γ_{small} and γ_{big} are set to 0.9. Finally ξ_{big} is 0.3 assuming approximately a third of the surface of big particles consists of broken cell walls. All Values are summarized in table 2

Variable	Value	Unit
m_{coffee}	10	g
ρ_{coffee}	400	kg/m^3
ζ_{coffee}	0.3	-
\bar{r}_{small}	39	μm
\bar{r}_{big}	550	μm
ν_{small}	0.25	-
ν_{big}	0.75	-
ζ_{small}	0.25	-
ζ_{big}	0.25	-
γ_{small}	0.9	-
γ_{big}	0.9	-
ξ_{big}	0.3	-

Table 2: values of model

With those values used for the modelling we get $\chi(t^* = 0) \approx 0.07$

5.2 Subsequent Phase

For the subsequent phase modelling there is also a set of variables to be quantified. First we consider the initial time to be approximately same as it takes to overcome the peak of the discharge. For a pressure difference of $\Delta p = 7 \text{ bar}$ we get $T_{init} \approx 1 \text{ s}$ from Fasano, Talamucci, and Petracco (2000).

Having T_{init} the starting time t^* of the chemical modelling is defined. With ζ_{coffee} already defined in the previous section the only open variable is τ which is needed to be tuned.

For that we first use our fit of the experimental discharge to get the time at which we reach the desired volume of $V_{coffee} = 30 \text{ ml}$. Since our discharge model neglects initial phase we need an approximate for the volume discharged before $t^* = 0$. From Fasano, Talamucci, and Petracco (2000) we get the mean initial velocity \dot{V}_{init} as 8 ml/s . Multiplying it with T_{init} we get $V_{coffee}(t^* = 0) = 8 \text{ ml}$. For the total volume of coffee we then use the results of the discharge modelling by integrating it:

$$V_{coffee}(t^*) = V_{coffee}(0) + \int_0^\infty \dot{V}_{coffee}. \quad (35)$$

From figure 12 we get $t^* = 35 \text{ s}$ for reaching the 30 ml goal.

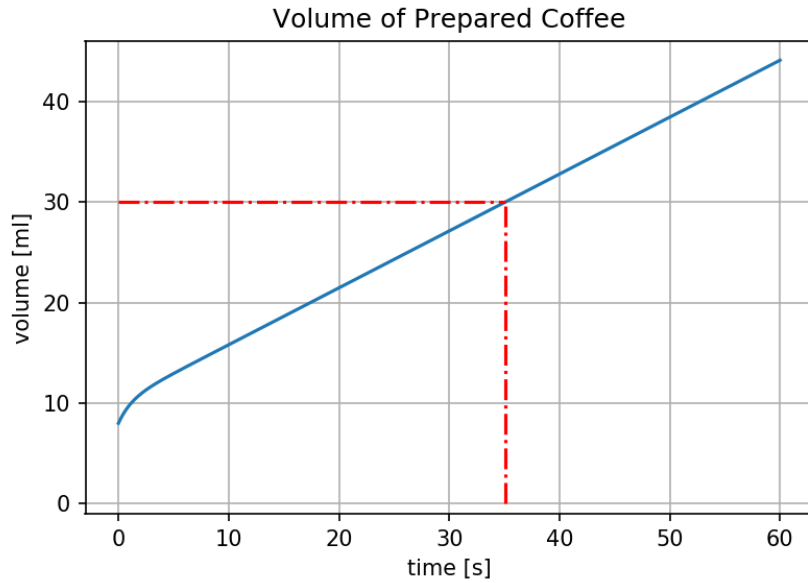


Figure 12: Volume of prepared coffee with $\Delta p = 7 \text{ bar}$

To have the perfect coffee and get the assumed perfect extraction yield of 25% proposed by Illy and Viani (2005) at $t^* = 35 \text{ s}$ we choose $\tau = 25 \text{ s}$. The course of extraction can be seen in figure 13.

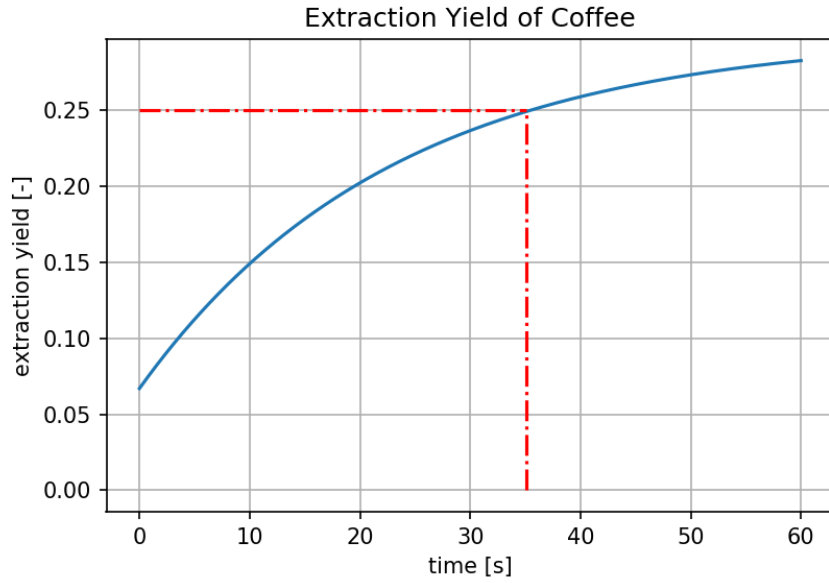


Figure 13: Extraction yield over time with $\Delta p = 7 \text{ bar}$

The proposed model is based on observations of underlying processes which makes it reasonable. Nevertheless there are several variables used whose values are only estimated due to the lack of experimental data. This leads to the assessment that this model cannot be seen as a predictive model for absolute values. Nevertheless it can be used to predict trends. Changes of operation parameters lead to a different discharge. This results in a different preparation time for $V_{coffee} = 30 \text{ ml}$. For $\Delta p = 5 \text{ bar}$ the preparation time is $t^* = 24 \text{ s}$ as can be seen from figure 14.

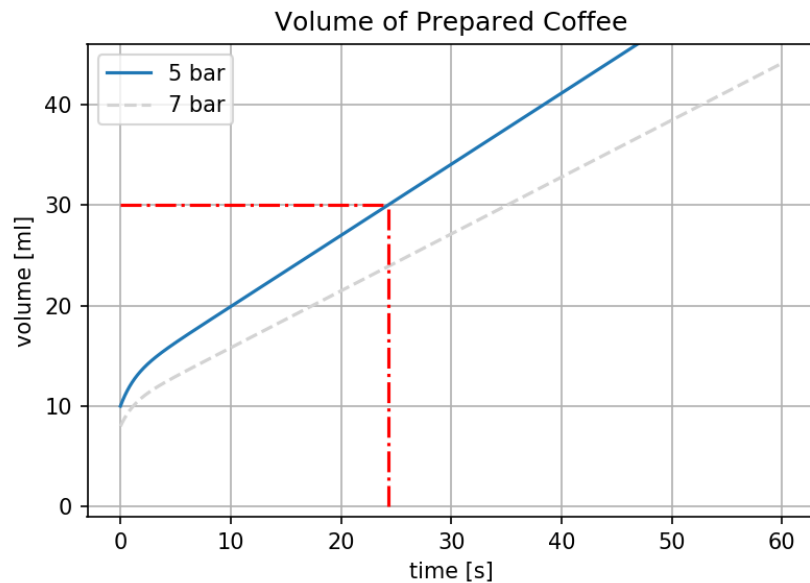


Figure 14: Volume of prepared coffee with $\Delta p = 5 \text{ bar}$

To reach the perfect extraction yield of $\chi = 25 \%$ an adaptation of τ is needed (compare figure 15).

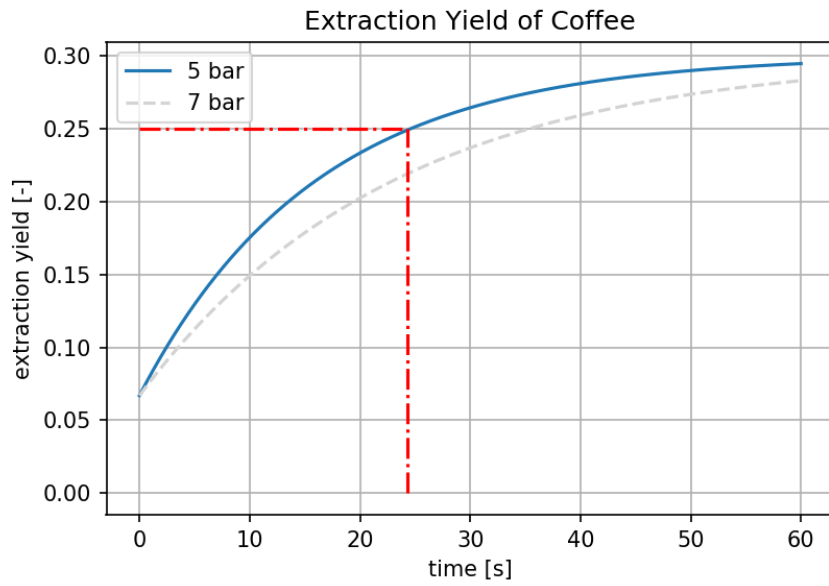


Figure 15: Extraction yield over time with $\Delta p = 5 \text{ bar}$

The new τ is now 16 s indicating the need of a much faster extraction process. Since τ is dependent on temperature, grinding process and machine's geometry we can adjust this parameters to reach a perfect espresso.

6 Discussion and conclusions

The mechanical model described in chapter 3 and the chemistry model discussed in chapter 4 fulfil the goal of the project to have basic models for the main aspects of the preparation of coffee. Nevertheless there are simplified assumptions made while developing the models. In chapter 5 the chemical model was applied to a set set of values. However due to a lack of information for some of the used variables this is not prescriptive. Also experimental data was used to determine the discharge of coffee. In a next step the mechanical model could be connected to the chemistry at that point. Finally while the mechanical modelling allows a deeper inside of the complex mechanics the happen in the coffee cake during preparation, the chemistry model is suitable for trend-forecasting and could be further optimised when experimental data was available.

7 Group work dynamics

Since the goal of the project was not fully predefined by the instructor group work started with defining own goals to reach within the Modelling Week. The separation of the problem into two distinctive modelling approaches allowed to split the group into subgroups. One pair was mainly working on the chemistry modelling while two pairs faced the mechanic modelling. Due to the complexity of the problem there was a high level of communication. Frequent summaries and discussions on the blackboard led to a higher understanding of the problem for all attendants. Also discussions with the instructor and an invited professor were very helpful. The lack of time within one week was limiting the complexity of the developed models, nevertheless by providing two modelling approaches we fulfilled our own goals. The high complexity of the problem and the parallel development of two models was a challenge but was also very interesting. The different study directions of the attendants sometimes complicated the communication but on the other hand led to a higher bandwidth of ideas. Writing the report was complicated by the previously distributed work. Collecting the output of every working pair and fit it into a coherent structure took some iterations. At the end we would like to point out that although the Modelling Week was challenging work but also a lot of fun and very instructive, both professional and also personal.

8 Instructor's assessment

Modelling the preparation of espresso-coffee is known to be a process which possesses extraordinary complexity. In brief, a stream of hot water is forced to flow through the bounded layer of coffee in granules. Afterwards it is collected in the cup. The flow of water (percolation) is accompanied by the extraction of soluble substance of coffee, as well as the transport of the solid phase which becomes the part of the coffee emulsion. The goal of the project was very general, to study the basic aspects of this process and to establish an appropriate mathematical model.

Due to the complexity of the problem, students separated in multiple groups on the first day. Although separated, they interacted very often and discussed achievements and problems they met in each group. Every student was present and active during the whole Modelling Week. The two main aspects of the problem were discussed, the mechanical and chemical part. Students consulted available literature, but also they built their own model, by specifying some possible – the simplest – submodels and numerically or analytically solving the corresponding equations. Therefore, we can say that the initial goal of the Modelling Week is achieved, with some perspectives, such as to consider more complicated submodels, and to improve chemical part of the problem.

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