Modelling swelling effects during coffee extraction with smoothed particle hydrodynamics

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It is commonly assumed that coffee particles swell during filtration, but it has not been clarified how different degrees of swelling affect the extraction. In this article, we propose a grain swelling model to investigate the influences of swelling on both intra-grain and inter-grain transport. The swelling is modelled through a diffusion process of excess water into the grains. The geometric expansion of the grains is connected to the local concentration of excess water through a specified deformation gradient tensor. Diffusion of soluble compounds inside the grains is coupled with the swelling dynamics through a modified diffusion equation. Inter-grain transport is modelled by solving the Navier-Stokes equation and diffusion equations. This model is solved numerically in the framework of smoothed particle hydrodynamics and it is used to simulate the extraction of a minimal coffee bed setup, and to investigate the effect of a small degree of particle swelling (< 8% in size) on the extraction kinetics. It is found that under the normal operating parameter regime of espresso filtration, swelling affects the extraction mainly through the change of inter-grain transport. Swelling also alters the diffusion inside the grains, but this process has a secondary effect on the extraction. In general, swelling slightly impedes the extraction rate, but enhances the strength considerably at both fixed brewing time and fixed brewing volume. Our results justify the endevour in the literatures to clarify the effect of possible swelling on brewing and preparation variables during coffee extraction.

I. INTRODUCTION

A coffee bed is a typical porous medium formed by packing millions of coffee particles. These coffee particles are produced by grinding roast coffee beans. During a grinding process, coffee beans break into small grains of an approximately bimodal size distribution. The first peak of the distribution function is always at around 30–40 µm, representing the so-called “fines”, i.e. inner walls cellular fragments. The second peak represents the so-called “coarses”, and its exact position depends on the grinder, with values ranging between 200µm ~ 1000µm. A third peak corresponding to submicron-scale particles might be present (“hyperfines”), but is relatively minor. Roast and ground coffee grains are not entirely solid. Cell-pockets of dimensions 30µm ~ 60µm form inside the grains after the destruction of biological cells during roasting. And the cell-walls are also porous at nanoscale. These make the roast ground grains a highly porous material. When a coffee is brewed, the porous coffee particles are wetted through a process called imbibition. During imbibition, the capillary pressure sucks water into the porous structure. It is known that roast coffee beans have much smaller contact angle than green coffee beans. As a consequence, the capillary pressure in roast coffee grains will be very high due to the small contact angle and small pore size, suggesting that the imbibition process might be very fast. Although the wetting of coffee particles could be fast, the actual swelling is a relatively slower process; according to Hargarten et al., the particle reaches 60%-80% of its steady-state diameter after 30s and the swelling completes after 4min of wetting.

There are three main polysaccharides comprising a coffee matrix: arabinogalactan, galactomannan, and cellulose. Cellulose is the only component that stays relatively constant throughout roasting. Hargarten et al. have observed that roasting degree does not affect the swelling and concluded that cellulose has the highest influence on swelling. In addition to cellulose, other β-(1,4) glycans, namely mannan fragments from thermally degraded galactomannan may also contribute to swelling. Depending on the structure of the microfibres and the solvent quality, cellulose can exhibit very diverse swelling and dissolution behaviours: fast dissolution by disintegration into fragments, large swelling by ballooning and complete dissolution, homogenous swelling, etc. However, the physical mechanism behind the swelling behaviour of roast coffee particle is still unclear. Dependence on water composition has been reported, as well as dependence on initial particle size. In addition, there is still no consensus on whether roast coffee particles swell during extraction and how much is the degree of swelling, if it does occur. The conclusion drawn by previous researchers varies from no swelling whatsoever to about 7% or 15% increase in size. The reason for these mixed opinions is that, the initial particle size, the degree of roast, and the water chemistry could all affect the process, making the problem difficult to solve. Finally, different measurement protocols using different inspection methods (microscopy and laser diffraction) could also introduce errors in the estimate of swelling degree.

In this article, we do not intend to resolve the debate on whether coffee particles swell during extraction, instead, we...
assume here that a small degree of swelling does actually happen, and investigate the effects of possible different swellings on the coffee extraction kinetics. Since the swelling of coffee particles affects the porous structure of the coffee bed, it will alter the permeability and it will be therefore influential on coffee extraction. However, it is unclear how this influence occurs and to what extent. Here, we intend to clarify this problem by simulating the percolation process with the swelling of coffee particles taken into account.

The study of flows through deformable porous media has drawn lots of attention due to its prevalence in nature and industry. In the field of paper and textile research, significant efforts have been devoted to clarify the interactions between fluid transport and the swelling of fibre networks. However, in the case of a porous medium formed by packing coffee particles, a particle-level swelling model is needed. There are only a few of these models in the literature. Mateus et al. considered an analytical solution of a diffusion equation for a spherical geometry to reproduce the swelling kinetics of a coffee particle. However, this model is inaccurate since it has to assume a fixed boundary to get the analytical solution while the boundary of a swelling sphere is moving. Studying the swelling of a superabsorbent polymer particle Sweijen et al. derive an approximate solution for the diffusion problem with the moving boundary taken into account. They use the solution to prescribe the evolution of particle diameter in a simulation of a bed of particles. The swelling kinetics can also be roughly described by a first-order expression based on Fick’s second law of diffusion as done in the work by Esteves. There is also an empirical swelling model that describes the evolution of the diameter of a swelling starch particle. However, all these models do not aim at the precise solution of the swelling dynamics of the grain. Moreover, they cannot be used to monitor the extraction dynamics of soluble compounds (trigonelline, caffeine, polysaccharides, etc) inside the particle and in the liquid phase. During a coffee percolation process, the extraction dynamics will be coupled with the swelling kinetics due the deformation of the particle.

Therefore, in order to study the coffee extraction problem with the particle swelling taken into account, in this article we propose a particle swelling model that properly considers the coupling between the deformation of the swelling particle and the intra-granular diffusion of water and other soluble compounds. We use this model to simulate the filtration of a minimal representative coffee bed in the framework of smoothed particle hydrodynamics (SPH), and investigate the effects of swelling on the extraction of coffee.

It is found that, despite the effect of the altered diffusion inside the grain is nearly negligible, the effect of the altered flow around the grains is much more significant. Under the normal operating parameter regime, the strength of the coffee will be considerably enhanced by a small degree of swelling at both fixed brewing time and fixed brewing volume.

The article is organised as follows. In section II the simulation models are introduced, including the SPH formalism (section II A), the porous medium model (section II B), the swelling model (section II C), the extraction model (section II D) and the single grain model (section III E). In section III the simulation results are presented, including the single grain simulations (section III A), the porous medium simulations (section III B) and the simulations considering the varying diffusion constant inside grains (section III C). Finally, conclusions are reported in section IV.

II. COMPUTATIONAL MODEL

A. Smoothed Particle Hydrodynamics formalism

In our model the flow is governed by the Navier-Stokes equations. To solve them, we employ the smoothed particle hydrodynamics (SPH) method, which is a particle-based hydrodynamics approach. SPH is derived through a Lagrangian discretisation of the Navier-Stokes equations. We employ an SPH version which conserves angular momentum, as it can be crucial for some problems. In SPH, each particle can be considered as a small fluid volume (or Lagrangian discretisation point) characterised by a position \( r_i \), velocity \( v_i \), and mass \( m_i \). In addition, each SPH particle possesses a spin angular velocity \( \psi_i \) and moment of inertia \( I_i \) introduced for the enforcement of angular momentum conservation.

SPH particles \( i \) and \( j \) interact through three pairwise forces, including conservative \( F_{ij}^C \), dissipative \( F_{ij}^D \), and rotational \( F_{ij}^R \) forces given by

\[
F_{ij}^C = \left( \frac{P_i}{d_i^2} + \frac{P_j}{d_j^2} \right) F_{ij} r_{ij},
F_{ij}^D = -\gamma_j \left[ v_{ij} + (e_{ij} \cdot v_{ij}) e_{ij} \right],
F_{ij}^R = -\gamma_i \frac{r_{ij}^2}{2} \times (\psi_i + \psi_j),
\]

where \( r_{ij} = r_i - r_j \), \( v_{ij} = v_i - v_j \), and \( e_{ij} = r_{ij}/r_{ij} \). Particle number density \( d_i \) is computed as \( d_i = \sum W_{ij} \) using a smoothing kernel function \( W_{ij} = W(r_{ij}) \) that vanishes beyond a cut-off radius \( r_c \) and defines a non-negative function \( F_{ij} \) through the equation \( W_{ij} = -r_{ij}/F_{ij} \). Then, particle mass density is given by \( \rho_i = m_i/d_i \). The pressure \( P_i \) is determined by the equation of state (EoS) \( P_i = P_0(d_i/d_0)^\nu - P_b \), where \( d_0 \) is the average number density, \( P_0 \) and \( \nu \) are parameters controlling the sound speed \( c = \sqrt{P_0\nu/d_0} \), and \( P_b \) relates to the background pressure. Furthermore, \( \gamma \) is a force amplitudes defined as

\[
\gamma_i = \frac{20\eta}{7} \frac{F_{ij}}{d_{ij}},
\]

where \( \eta \) is the fluid dynamic viscosity.

The evolution of particle positions, translational and angular velocities is obtained by integration of the following equations of motion

\[
r_i = v_i, \quad m_i \dot{v}_i = \sum_j F_{ij} = \sum_j (F_{ij}^C + F_{ij}^D + F_{ij}^R), \quad \dot{\psi}_i = \frac{1}{2I_i} \sum_j r_{ij} \times F_{ij},
\]

where \( I_i \) is the moment of inertia.
using the velocity-Verlet algorithm\textsuperscript{34}\textsuperscript{35}. In this work, the smoothing kernel is represented by the quintic spline kernel function\textsuperscript{35}:

\[
W(q) = w_0 \begin{cases} 
(3-q)^3 - 6(2-q) + 15(1-q)^2, & 0 \leq q < 1 \\
(3-q)^3 - 6(2-q), & 1 \leq q < 2 \\
(3-q)^3, & 2 \leq q < 3 \\
0, & q \geq 3 
\end{cases}
\]

where \( q = r/h \) and \( w_0 = 1/(120\pi h^3) \) in three dimensions (3D), \( w_0 = 7/(478\pi h^2) \) in two dimensions (2-D), and \( h \) is the smoothing length \( h = r_c/3 \).

B. Porous medium model

A realistic coffee bed is normally a couple of centimetres in height and consists of millions of individual coffee grains “coarse”), and it is therefore technically difficult to model it at microscale resolution. Since the main aim of this work is to show the effects of swelling, it can be achieved through the modelling of a representative mini-bed consisting of several dozens of grains. A schematic for the porous medium model representing a mini-bed is shown in Fig. 1. The simulation box is a 3-D box of size \( L_x \times L_y \times L_z \). At the lower part of the box, 40 grains (whose size is uniformly distributed 2 \( \leq R \leq 4 \)) are packed randomly to form a porous medium. \( L_z \) is the distance between the initial level of the fluid and the bottom of the box, which will increase with the swelling of the grains. Both the fluid and the solid are discretised using SPH particles (see Fig. 1). The SPH particles forming each solid grain are interconnected using stiff harmonic bonds:

\[
F_{ij}^B = -k_b(l_{ij} - \ell_{ij}^0),
\]

where \( l_{ij} \) is the bond length and \( \ell_{ij}^0 \) is the equilibrium bond length, \( k_b \) is the spring coefficient. To avoid the consolidation problem and also to prevent the solid grains from moving across the vertical boundary, the grains are tethered by stiff springs to their original centres of mass:

\[
F_j^s = -k_s(r_j^{cm} - R_j^{cm}),
\]

where \( r_j^{cm} \) is the position vector of the centre of mass of the \( j \)-th grain, \( R_j^{cm} \) is its initial position vector, \( k_s \) is the coefficient of the tethering spring.

A downward body force \( g \) is applied to all the particles and drives the fluid through the porous medium. All boundaries are periodic. A fluid particle that has moved across the lower boundary will be reinserted on the top, but with the concentrations of compounds being reset as it will be explained in the next section.

C. Swelling model

At the start of the filtration, the coffee grains are wetted rapidly by capillary action: micro-pores on the coffee grains and nano-pores on the cell walls imbibe the water by capillary force. This imbibition process can be approximately described by the classical Washburn equation or by solving N-S equations numerically together with the volume of fluid method\textsuperscript{36}. During the imbibition process, water molecules may also combine with the hydroxyl groups in the cellulose fibre, and cause the porous matrix to expand. In principle, imbibition and swelling happen at the same time, and will influence each other, rendering the Washburn equation inaccurate. In the industry of paper-making, researchers have developed mathematical models\textsuperscript{37,38} to try to consider the coupling between imbibition and swelling. But to the best of our knowledge, no effort has been made to model the coupling process of imbibition and swelling of coffee particles. This is justified by the fact that the imbibition process of a coffee particle lasts only a couple of seconds\textsuperscript{37,38} given its very small size, while the swelling process is much slower. Experimental studies suggest that the swelling completes in 4min after wetting\textsuperscript{6}. Therefore, in this article, we will also assume that the initial wetting occurs instantaneously and does not affect the subsequent swelling process.

We model the swelling process as a diffusion process of excess water into the grain combined with a concomitant expansion of the geometry. Our approach is similar to that of Sweijen et al\textsuperscript{15} and Mateus et al\textsuperscript{24} where the swelling of a grain particle is assumed to be governed by the diffusion of water into the grain. However, differently from the analysis method of Sweijen et al\textsuperscript{15}, where two separate phases (fluid and solid) are considered, here we consider a solid phase whose water concentration can be varied and its geometry can expand according to a specified constitutive relationship. We solve the diffusion-swelling coupled equation precisely, rather than using an approximate solution like Sweijen et al\textsuperscript{15} and Mateus et al\textsuperscript{24}. The excess water concentration \( c^w(x,t)[L^3/L^3] \) is defined to be the volume percentage of excess water inside a particle element. We assume the swelling to be isotropic, and the relationship between the deformation of the solid and the excess water concentration is specified as:

\[
\frac{dx}{d\mathbf{X}} = F = [1 - c^w(x,t)]^{-1/d_n} \mathbf{I},
\]

where \( \mathbf{X} \) is the position of a material point of the grain before swelling, \( x \) is the position of this point after swelling, \( \mathbf{F} \) is the deformation gradient tensor, \( d_n \) is the dimension of the problem.

The governing equations for the swelling process reads therefore:

\[
\frac{\partial c^w(x,t)}{\partial t} = D^w \Delta c^w(x,t) - \frac{\partial J(x,t)}{\partial t} \frac{\partial c^w(x,t)}{\partial J(x,t)}, \quad \text{for } \mathbf{X}(x,t) \in \Omega_0
\]

where \( D^w[L^2T^{-1}] \) is the diffusion coefficient of water inside the grain assumed to be constant, \( J \) is the volume transformation factor \( J = \det(F) = 1/[1 - c^w(x,t)] \), \( \Omega_0 \) is the domain of the grain at \( t = 0 \). The first term on the right hand side accounts for the diffusion contribution, while the second term accounts for the contribution due to the swelling of the solid volume. Inserting the expression of \( J \) into the above equation yields:
\[
\frac{dc^w(x,t)}{dt} = D^w \left[ 1 - c^w(x,t) \right] \Delta c^w(x,t), \quad \text{for } X(x,t) \in \Omega_0
\] (9)

This equation is subject to the initial conditions:
\[
c^w(x,0) = 0, \quad \text{for } X(x,0) \in \Omega_0
\] (10)
\[
x = X, \quad \text{for } t = 0
\] (11)

and boundary conditions:
\[
c^w(x,t) = 1, \quad \text{for } X(x,t) \in \Gamma_0,
\] (12)
\[
x(x,t) = g(t), \quad \text{for } X = X_0,
\] (13)

where \( \Gamma_0 \) is the boundary of the grain at \( t = 0 \), \( X_0 \) is a point inside the grain, \( g(t) \) is a known function accounting for the rigid displacement for the grain.

This description of the swelling dynamics can be straightforwardly discretised using the SPH method. First the geometry is discretised using SPH particles as shown in Fig. 1.

Equation (8) is then discretised and reads:
\[
\frac{dc^w}{dt} = \sum_j \left[ F^w_{ij} \frac{D^w}{r_{ij}d_i} + F^w_{ij} \frac{D^w}{d_j} \right] W_{ij} c^w_{ij}
\] (14)

Note that the second term on the RHS of Eq. (8) will be accounted for by the deformation of the grain given below. The boundary condition is imposed by setting \( c_i^w = C_M \), with \( C_M \) being the maximum excess water concentration of the grain, for all surrounding fluid particles.

To account for the deformation caused by swelling, the solid SPH particles are interconnected by harmonic bonds as shown in Fig. 1 and the equilibrium length of the harmonic bonds are varied according to the local excess water concentration. We need to integrate Eq. (7) to get the updated bond equilibrium length:
\[
x_{ij} = \int_{X_i}^{X_j} \left[ 1 - c^w(X) \right]^{-1/\alpha_n} dX
\] (15)

This can be simplified to be
\[
\ell_{ij}^0 = \begin{cases} 
\ell_{ij}^0 \frac{1}{c_i^w - c_j^w} \log \frac{1-c_i^w}{1-c_j^w}, & \alpha_n = 1 \\
\ell_{ij}^0 \frac{(1-c_i^w)^{1-\alpha_n} - (1-c_j^w)^{1-\alpha_n}}{(c_i^w - c_j^w)^{1-(1-\alpha_n)}} & \alpha_n > 1
\end{cases}
\] (16)

where \( \ell_{ij}^0 \) is the equilibrium length of the bond between particle \( i \) and \( j \), and \( \ell_{ij}^0 \) is the equilibrium length of the bond before any swelling. To prevent the liquid SPH particles from penetrating into the solid domain, the pressure \( P_l \) in Eq. (1) for the solid particles is fixed as \( P_l = P_0 - P_b \). This trick will not work if the swelling degree is too high, therefore our method cannot be used to model the swelling of superabsorbent polymers. Note that we have used a phase different from the fluid phase around the coffee particles to model the excess water inside the coffee particle. If we had modelled the excess water using the same SPH particles around the grains we would have constrained the resolution of the excess water to be the same as the SPH particle resolution and could not have described swelling of very small degree. According to our simulation the swelling can be as large as \( \approx 20\% \) in size without causing the fluid SPH particles to penetrate into the solid phase. However, it is unlikely that coffee particles can really swell to such a degree. Experimental measurements on the swelling degree of coffee particles range from no swelling at all to 15% of swelling in size\(0.13-1.5\). In this article we consider only a moderate degree of swelling (\(<8\%\)).

In our SPH model, during swelling the fluid SPH particles do not actually enter into the solid domain, only another phase of excess water (which has a much higher resolution) enters into the solid domain and expands the volume of the solid. This leads to an increase of the total volume of the solid and fluid domains and is a limitation to our SPH model. The physical meaning of this limitation is that we cannot set the absorption coefficient \( b \) (which is defined in Pillai’s work\(23\)) to
be 1 as classical swelling models did. But in reality this absorption coefficient is not necessarily to be 1 due to more complicated multiphase effects (e.g. gas trapped in the microscopic intra-grain close pores). Nevertheless, because this limitation only slightly affects the flows around the coffee particles, while the downward flow due to the applied external pressure is much stronger it will not affect our main conclusions on the extraction kinetics.

Finally, the maximum swelling degree \( s_m \) is related to the maximum excess water concentration by:

\[
s_m = \frac{r_{\text{max}}}{R} - 1 = ((1 - C_M)^{-1/d_0} - 1) \times 100% , \tag{17}\]

where \( r_{\text{max}} \) is the maximum radius of the coffee particle.

### D. Extraction model

Let’s consider some kind of soluble compounds (trigonelline, caffeine, polysaccharides, etc) that is extracted from the grains to the fluid. Inside the grain, the diffusion of the soluble compound \( c \) is coupled with the diffusion of excess water \( c^w \) through the swelling effect:

\[
\frac{\partial c}{\partial t} = \nabla \cdot (D_p \nabla c) - c D^w \Delta c^w. \tag{18}\]

The diffusion constant \( D_p \) is an average over the porous and heterogeneous structure inside the coffee particle. It can be estimated by \( D_p = D_h/(H_g H_j)^{39} \), with \( D_h \) being the diffusion constant in the bulk of water, \( H_g \) being the geometric hindrance factor, and \( H_j \) the solute hindrance factor. \( H_j \) can be estimated as \( H_j = \beta_p/\varepsilon_p^{40} \), with \( \varepsilon_p \) being the average porosity inside the particle, and \( \beta_p \) the average intra-particle tortuosity. The swelling effect will cause \( \varepsilon_p \) to increase, altering \( D_p \). We can simply assume that \( H_g \) is constant since we are considering only a very small degree of swelling (< 8%). In that case, we set \( H_g = 8 \), and \( H_j = 4 \) following some experimental measurements.\[13,39\] We can also take the varying \( H_g \) into account with

\[
H_g = H_g^0 / (1 + (1 - e_0^p)/(e_0^p - e^w)), \tag{19}\]

where \( e_0^p \) is the initial particle porosity before swelling, \( H_g^0 \) is the initial geometric hindrance. In that case, we set \( e_0^p = 0.5 \), \( H_g^0 = 8 \), following experimental measurements.\[13\]

Equation (13) can be discretised in the SPH framework as:

\[
\frac{dc_i}{dt} = \sum_j \frac{(D_p d_i + D_p d_j) W_{ij}}{r_{ij} d_i d_j} \cdot \nabla \cdot \nabla c. \tag{21}\]

In SPH, the convection term is already accounted by the migration of the Lagrangian particles, so only the diffusion term is present in the discretised form:

\[
\frac{dc_i}{dt} = \sum_j \frac{(D_p d_i + D_p d_j) W_{ij}}{r_{ij} d_i d_j} \cdot \nabla \cdot \nabla c. \tag{22}\]

The transport of soluble compound between liquid/solid interfaces is modelled using a uni-directional diffusion process:

\[
\frac{dc_i}{dt} = \sum_j \frac{(D_p d_i + D_p d_j) W_{ij}}{r_{ij} d_i d_j} \cdot \nabla \cdot \nabla c. \tag{23}\]

where \( D_p \) is the release coefficient.\[12\] We specify \( D_p^j = D_p \) if particle \( i \) and \( j \) are in different phases, and the concentration in the solid phase is higher than that in the liquid phase, otherwise \( D_p^j = 0 \).

In the porous medium model (Fig. 1), the boundaries in the \( y \) direction have to be handled specially for the extracted compound. For the fluid particles, they can move across the lower \( y \) boundary and reappear at the upper \( y \) boundary, but when this crossing happens, the concentration of the fluid particles will be reset to zero. Diffusion across the boundary in the \( y \) direction is also not allowed. These guarantee that the water entering from the upper boundary is always “fresh” water.

### E. Single grain model

In order to validate the model, we consider first the simple case of a single grain. As shown in Fig. 2 only one coffee particle with spherical symmetry is explicitly modelled. The boundaries in the \( x \) and \( z \) directions are periodic but the boundary in the \( y \) direction is impenetrable. Therefore the flow rate will always be \( V = 0 \), leading to a Peclet number: \( \text{Pe} = 2RV/D_h = 0 \). However, if in the simulation we reset the concentration of all the fluid particle to be \( c_i = 0 \) at every time step, for the grain it is equilibrium to have \( V = \infty \) i.e. \( \text{Pe} = \infty \). Therefore, using this simple model we can illustrate how the swelling affects the extraction of soluble compounds from the grain in two extreme conditions: \( \text{Pe} = 0 \) and \( \text{Pe} = \infty \). In the case of \( \text{Pe} = \infty \), the fluid can flush away the extracted compound as soon as the compound diffuses out of the grain. On the contrary, in the case of \( \text{Pe} = 0 \), the diffused compound accumulates around the grain, altering the boundary condition of the diffusion inside the grain. In our single grain model, the initial porosity is set 0.66, and it will decrease when the grain swells. The porosity is irrelevant for \( \text{Pe} = \infty \), however, when \( \text{Pe} = 0 \), it represents how much fluid there is to absorb the soluble compounds, and thus it will affect the extraction dynamics.

### F. Implementation and simulation parameters

We implement the SPH method, the porous medium model, the swelling model, and the extraction model by modifying
the source code of the classical open source molecular dynamics software LAMMPS.

The basic SPH parameters are summarised in Table I. If not explicitly specified, values in the table are used. Parameters for the single grain simulation are summarised in Table II. Parameters for the porous medium simulation are summarised in Table III. In these tables, both the numerical values used in the simulation and their corresponding values in SI units are presented. The values in SI units are obtained as follows. First we select three base parameters with independent dimensions. Then we specify the scaling relationship of these parameters with their values in SI units. Finally, all other parameters can be scaled to the SI units using these three base parameters. Here we use the cutoff radius, the mass density and the dynamic viscosity as base parameters. Their values in SI units are first specified as in Table I, the values of all other parameters in SI units are determined accordingly. The result is shown in the last column of the tables. Note that if we choose different values in SI units for the three base parameters the model can be scaled to many different prototypes. But all these prototypes and the numerical model are physically similar, since the dimensionless parameters (Reynolds and Peclet numbers) are identical. We can also change the choice of base parameters and many other prototypes can be obtained. For example we can choose the grain diameter, the diffusion coefficient and the mass density as base parameters and always specify their values in SI units to be in agreement with the realistic values. It is just for consistency and simplicity that we have fixed the base parameters as the cutoff radius the mass density and the viscosity.

In Table III we increase the coefficient of diffusion to decrease the Pe number, rather than only decrease the flow rate. This seems to be unphysical but it has the advantage of saving computation time significantly. And because the governing dimensionless parameters are the Reynolds and Peclet numbers, as long as these two numbers have the values we want the simulation result always represents the right prototype we target.

### III. RESULTS AND DISCUSSION

#### A. Results for the single grain simulation

We first examine the swelling dynamics. In a spherical coordinate system, the governing equation Eq. 9 reduces to:

$$
\frac{\partial c^w}{\partial t} = D^w (1 - c^w) \frac{1}{R^2} \left[ \frac{4r^2}{R^2} \frac{\partial c^w}{\partial R} - \frac{2r^4}{R^4} (1 - c^w) \frac{\partial ^2 c^w}{\partial R^2} - \frac{r^4}{R^2} (1 - c^w) \frac{\partial ^2 c^w}{\partial R^2} + \frac{r^4}{R^2} (1 - c^w) \frac{\partial ^2 c^w}{\partial R^2} \right], \text{ for } R < \mathcal{R},
$$

with

$$
r^3 = 3 \int_0^R \xi \left[ 1 - c^w(\xi) \right]^{-1} d\xi.
$$

The initial condition and boundary condition are:

$$
c^w(R,t=0) = 0, \text{ for } R < \mathcal{R},
$$

The above equations can be solved using the finite difference method, an example is shown in Fig. S where we have set

$$
\frac{\partial c^w}{\partial R} = 0, \text{ for } R = 0.
$$

![FIG. 2: (a) Schematic of single grain model. (b) SPH representation of the single grain model.](image-url)
$R^2/D_w = 10s$, $C_M = 0.2$. Figure 5(a) shows how the excess water inside the grain evolves with the water absorption and swelling progressing. The arrow denotes the evolution direction. As can be seen from the figure, at the beginning, excess water only enters the grain at the boundary, we have a very stiff concentration curve. As more water diffuses into the grain, the concentration curve becomes smooth, concentration at the centre also increases. At $tD^w/R^2 = 0.4$ the concentration of excess water inside the grain almost becomes uniform and is close to the uptake limit $C_M = 0.2$. Figure 5(b) shows the concomitant expansion of the grain radius. The corresponding contours of the excess water inside the grain at several selected instants ($tD^w/R^2 = 0.1, 0.2, 0.3$) are also presented in Fig. 5. In Fig. 5(b) we have also shown the results predicted using Sweijen’s formula:

$$\frac{dQ_{abs}}{dt} = \frac{3D^w}{\alpha R^3} \left( \frac{Q_{max} - Q_{abs}}{Q_{abs}} \right)$$

(30)

and the formula reported in Esteves’s work:

$$\frac{dQ_{abs}}{dt} = \frac{\pi^2 D^w}{R^2} \left( \frac{Q_{max} - Q_{abs}}{Q_{abs}} \right),$$

(31)

where $Q_{abs} = r^3/R^3$ is the absorption ratio (we assume that the density of the liquid and the solid is the same), and $Q_{max}$ is the maximum of $Q_{abs}$. In the Sweijen’s formula, there is a free parameter $\alpha$. The physical meaning of $\alpha r$ is the distance from $r$ to a location inside the grain at which the excess water concentration is equal to the average concentration. We try both $\alpha = 1.0$ and $\alpha = 0.3$ in Fig. 5(b). As it can be seen, the numerical result of our current model is close to the result using Sweijen’s formula with $\alpha = 0.3$ and the formula from Esteves’s work. It should be bear in mind, however, that our model is more accurate since we have solved the problem precisely rather than trying to obtain an approximate analytical solution as in Sweijen’s work.

By setting $R^2/D_w = 40s$, and $C_M$ varying from 0.05 to 0.2, we compare the finite difference results with the SPH results in Fig. 5C showing good agreement. The slight difference originates from the fact that in Eq. (7) it is assumed that a solid element can swell freely and is not affected by its neighbouring elements. This assumption is invalid when the swelling degree varies fast across the grain. If the grain does not swell uniformly those parts swelling slower will hinder the other parts that swell faster. Our SPH model can take this effect into account, and that is the reason why in Fig. 5C the swelling rates from the SPH simulation are slightly lower than the finite difference results.

Next, we examine the extraction process. Since here the flow rate is assumed to be either zero or infinity, there are only two relevant time scales: the swelling time scale $T_s = R^2/D_w$ and the diffusion time scale $T_d = R^2/D_p$. The dimensionless quantity that controls the swelling and diffusion dynamics is therefore $T_s/T_d$. It has been reported that the time scale of water absorption into the coffee grain compares well with the time needed for most of the soluble compounds to be released. Therefore we focus on the cases $T_s/T_d \sim 1$ in our simulations. The geometric hindrance $H_g$ is fixed con-

<table>
<thead>
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<th>Values in SI units</th>
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<td>Dynamic viscosity $\eta$</td>
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<td>0.054 ms</td>
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<table>
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<th>Parameters</th>
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<td>Initial radius of the grain $R$</td>
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<td>Diffusion coefficient of the compound in liquid phase $D_0$</td>
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<td>L$^2$T$^{-1}$</td>
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<tr>
<td>Initial geometric hindrance factor $H_g$</td>
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<td>8</td>
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<tr>
<td>Solute hindrance factor $H_s$</td>
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<td>$C_M \in {0,0.05,0.1,0.2}$</td>
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TABLE III: Model parameters for the porous medium simulations.

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<td>Initial height of the liquid level $L_s$</td>
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<td>Initial radius of the grains $\mathcal{R}$</td>
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<td>$L \times 113 \mu m \leq \mathcal{R} \leq 226 \mu m$</td>
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<tr>
<td>Initial geometric hindrance factor $H^0_g$</td>
<td>$8$</td>
<td>$1 \times 8$</td>
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<tr>
<td>Solute hindrance factor $H_c$</td>
<td>$4$</td>
<td>$1 \times 4$</td>
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<tr>
<td>Initial intra-grain porosity $\varepsilon^0_0$</td>
<td>$0.5$</td>
<td>$1 \times 0.5$</td>
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<tr>
<td>Maximum excess water concentration $C_M$</td>
<td>$C_M \in {0, 0.05, 0.1, 0.2}$</td>
<td>$1 \times C_M \in {0, 0.05, 0.1, 0.2}$</td>
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<tr>
<td>Coefficient for the tethering springs $k_g$</td>
<td>$160000$</td>
<td>$\text{MT}^{-2} \times 3.4 \text{mN/m}$</td>
</tr>
</tbody>
</table>

Case 1 (High Pe number)

Downward body force $g$ on each SPH particle | $8.0$ | $\text{MLT}^{-2} \times 9.6 \times 10^{-12} \text{N}$ |
Diffusion coefficient for the water $D^w$ | $0.002$ | $\text{L}^2 \text{T}^{-1} \times 2.4 \times 10^{-10} \text{m}^2/\text{s}$ |
Diffusion coefficient of the compound in liquid phase $D_b$ | $D_b \in \{0.032, 0.064\}$ | $\text{L}^2 \text{T}^{-1} \times \{3.84 \times 10^{-9}, 7.68 \times 10^{-9}\} \text{m}^2/\text{s}$ |

Case 2 (Low Pe number)

Downward body force $g$ on each particle | $4.0$ | $\text{MLT}^{-2} \times 4.8 \times 10^{-12} \text{N}$ |
Diffusion coefficient for the water $D^w$ | $0.04$ | $\text{L}^2 \text{T}^{-1} \times 4.8 \times 10^{-9} \text{m}^2/\text{s}$ |
Diffusion coefficient of the compound in liquid phase $D_b$ | $D_b \in \{0.64, 1.28\}$ | $\text{L}^2 \text{T}^{-1} \times \{7.68 \times 10^{-8}, 1.54 \times 10^{-7}\} \text{m}^2/\text{s}$ |

FIG. 3: (a) Excess water concentration inside the grain during swelling process. The arrow marks the evolution direction. Warmer colours represent results at later times during the swelling process. (b) Evolution of the radius of the swelling grain. The finite difference result is compared with the results using Sweijen’s formula and the formula reported in Esteves’s work (Eq. 30 and Eq. 31). The dash line marks the swelling limit determined by $(1 - C_M)^{-1/3}$.

FIG. 4: A swelling grain. Contours inside the grain represent the concentration of excess water. (a) $tD^w/R^2 = 0$; (b) $tD^w/R^2 = 0.1$; (c) $tD^w/R^2 = 0.2$; (d) $tD^w/R^2 = 0.3$. 

(a) (b) (c) (d)
FIG. 5: Evolution of the grain radius at different maximum excess water concentration \( C_M \). Solid line: finite difference results; Circles: SPH results; dash lines: maximum swelling degree at different \( C_M \).

For \( Pe = \infty \), the more complicated case where \( H_g \) decreases with swelling will be discussed later. The SPH results for \( Pe = \infty \) and \( Pe = 0 \) are shown in Fig. 6. In that figure, we have fixed the swelling timescale \( T_s \) and \( T_d \) so that \( T_s/T_d = 1 \) and the maximum swelling degree is varied from 0 to 7.7% (corresponding to \( C_M \) varying from 0 to 0.2). The yield, or the extraction efficiency, is defined as the content that has been extracted out of the grain divided by the initial content inside the grain:

\[
\text{Yield of a single grain} = \frac{\int_{\Omega} c(t = 0, \mathbf{r}) \, d\mathbf{r} - \int_{\Omega} c(t, \mathbf{r}) \, d\mathbf{r}}{\int_{\Omega} c(t = 0, \mathbf{r}) \, d\mathbf{r}} \times 100\% ,
\]

(32)

where, \( \Omega (t) \) is the solid domain of the grain at time \( t \). Therefore the slope of the curves in Fig. 6 represents the rate at which the compound is extracted out of the grain. We can see from the figure that the swelling have indeed some effects on the extraction efficiency, that is swelling slightly impedes the extraction. When the flow rate around the grain is very fast, the effect of the swelling is slightly larger than when the flow rate is zero. In any case, the effect of the swelling on the extraction efficiency is quite small here. Notice that, in the single grain model, we have assumed that the swelling does not affect the flow rate. This assumption is not met in reality: since the packed bed of coffee grain will be affected by the swelling of the grains. The porosity and the permeability will be affected, and so does the local flow rate. This is the reason why simulations with the full porous medium are needed.

B. Results for the porous medium simulation

For the porous medium simulation, the Reynolds number is defined as \( Re = 2 \bar{R} \nu_s / \eta \), and the Peclet number is \( Pe = \nu_s \bar{R}^2 / D_b \), with \( \nu_s \) being the superficial flow rate and \( \bar{R} \) being the average radius of the grains. For a typical Italian espresso, 25ml of water is pushed through a 7g coffee bed in about 25 seconds. Consider a single filter basket whose diameter is about 6cm, the superficial flow rate will be \( 3.5 \times 10^{-4} \text{m/s} \). If we assume that the typical diameter of the coffee grains ("coarse") is around 340\( \mu \text{m} \), the Reynolds number for the filtration will be 0.12. Soluble compounds released from the coffee grains has a diffusion coefficient around \( 2 \times 10^{-9} \text{m}^2/\text{s} \) in liquid phase (dependent on the specific compound, concentration and temperature). This definition of the dimensionless numbers gives us a Peclet number around 60. However, due to the erosion inside the coffee bed, channelisation will happen in the medium, and some regions of the medium will have much smaller flow rate. The Reynolds and Peclet number will be significantly smaller in those regimes. Therefore, we perform two case studies: one is with both relatively large Reynolds and Peclet numbers, and the other with relatively small Reynolds and Peclet numbers. The SPH simulation setup and a typical result showing the trajectories of fluid particles through the porous medium are presented in Fig. 7.

Again, we fix \( T_s/T_d \sim 1 \). The geometric hindrance \( H_g \) is also fixed constant \( H_g = H_g^0 \). The first case is with \( Re = 0.14 \). Here, since the flow rate changes as a result of the swelling, the initial flow rate is used to determine the Reynolds number. We examine different maximum swelling degree \( s_m \) by varying \( C_M \). The evolutions of the total grain volume, the porosity, the superficial flow rate, and the yield are shown in Fig. 8. The yield for the coffee bed is defined as

\[
\text{Yield of the bed} = \frac{\int_{\Omega_s} c(t = 0, \mathbf{r}) \, d\mathbf{r} - \int_{\Omega_s} c(t, \mathbf{r}) \, d\mathbf{r}}{\int_{\Omega_s} c(t = 0, \mathbf{r}) \, d\mathbf{r}} \times 100\% ,
\]

(33)

where \( \Omega_s \) is the whole domain of the simulation box which is fixed. As can be seen from Fig. 8(a) and (b), the volume and the solid grains increase due to the swelling, the porosity of the bed decrease accordingly. Since the pressure drop is fixed,
FIG. 7: (a) SPH simulation setup. (b) Trajectories (unwrapped) of fluid particles through the swelling porous medium.

FIG. 8: Swelling and extraction with Reynolds number $Re = 0.14$ and high Peclet number. (a) Evolution of the total volume of the grains. The dash black lines mark the maximum swelling degrees. (b) Porosity of the medium. (c) Superficial flow rate. (d) Extraction efficiency. For the solid lines $Pe = 18.23$, $T_s/T_d = 1$, for the dash lines $Pe = 36.46$, $T_s/T_d = 0.5$.

If we use the initial flow rate to determine the Peclet number, $Pe = 18.23$ for the solid lines and $Pe = 36.46$ for the dash lines. As it can be seen, the swelling does have some effects on the extraction rate: a larger swelling degree slightly impedes the extraction. However, the effect is very small, just as in the

the flow rate also decrease with swelling as shown in Fig. 8 (c). Higher degree of swelling results in larger decrease of flow rate. Fig. 8 (d) shows the yield of two compounds. The diffusion coefficient for the one represented by the dash lines is half of that of the compound represented by the solid lines.
single grain simulation. The reason for this is simple: at high Peclet number, the fluid around the grains absorbs and flushes the compound so fast that a little variation of the flow rate does not alter the results. The swelling affects the yield through two ways: firstly, swelling slightly impedes the diffusion inside the grains as shown in the single grain simulation; secondly, swelling decreases the flow rate, therefore reducing the ability of the fluid to flush away the compounds. At the limit of Pe = ∞, swelling affects the extraction only through its influences on the diffusion inside the grains, while this influence is quite small.

The second case studied is at small Re = 0.068. The results are shown in Fig. 9. The evolutions of the solid volume, the porosity and the flow rate are similar to the previous case. In Fig. 9(d) the Peclet number is Pe = 0.44 for the solid lines, and Pe = 0.88 for the dash lines. Again, the diffusion coefficient for the one represented by the dash lines is half of that of the compound represented by the solid lines. We see that, the influence of swelling here is much larger. That is because when the Pe is small, the flow rate will be more influential on the extraction efficiency. Swelling reduces the flow rate, causing the extraction to also decrease accordingly. Interestingly, in the previous case with large Pe the diffusion coefficient inside the grain is very influential, but here the same parameter has only slight effects on the extraction rate. The explanation for this is connected to what the main factor constraining the extraction is. At high Pe the ability of the fluid to flush away the compound is very strong, and it is the slow diffusion inside the grain that hinders the extraction. As a result, the effect of the value of the intra-granular diffusion coefficient is very large. On the other hand, when Pe is small, it is the slow flow rate around the grains that hinders the extraction, and therefore increasing or decreasing the diffusion coefficient will not change the outcome significantly.

The curves of the yield are plotted against the brewing time, and they only reflect how fast the compounds are extracted. On the other hand, the taste and aroma of the coffee can be better characterised by the beverage strength, which is defined as the ratio between the mass of the extracted compound and the total fluid mass in the cup:

$$\text{Strength} = \frac{\int_{\Omega_t} c(t=0, \mathbf{r}) - \int_{\Omega_t} c(t, \mathbf{r})}{\int_0^t Q(\tau) \rho_0 d\tau} \times 100\%,$$

where $Q$ is the flow rate in volume, $\rho_0$ is the density of the liquid, $\rho_{\text{compound}}$ is the density of the compound, $\Omega_t$ is the whole domain of the simulation box. Referring to the density of caffeine in arabica coffee beans, we assume that $\rho_{\text{compound}} = 0.012 \rho_0$. The beverage strength for the two cases studied above are presented in Fig. 10(a) and (b). As can be seen, at both high and low Peclet number swelling has a significant effect on the strength. In general, swelling in-
FIG. 10: Strength for the two studied cases. (a) $Re = 0.14$, for the solid lines $Pe = 18.23$, for the dash lines $Pe = 36.46$. (b) $Re = 0.068$, for the solid lines $Pe = 0.44$, for the dash lines $Pe = 0.88$. (c) and (d) are the same results as (a) and (b) but shown against the total fluid volume in the cup $Q_{acc}$ (normalised by the volume of the porous medium $V_{bed}$).

FIG. 11: Extraction efficiencies for a single grain with the hindrance factor $H_g$ affected by swelling. Solid lines: $Pe = \infty$, dash lines: $Pe = 0$.

increases the strength due to the reduced flow rate. However, in the case of small Peclet number the effect of the swelling on the strength is only significant after $tD^w/\bar{R}^2 > 0.5$, that is, after the grains have fully swelled. It is also interesting to note that at low Pe the diffusion coefficient is only influential in the transient swelling stage ($tD^w/\bar{R}^2 < 0.5$), after that time, the curves with different diffusion coefficient but the same swelling degree tends to converge.

We have compared the outcomes with different swelling degree at the same brewing time, but due to the influence of the swelling on the permeability, the fluid volume in the cup will be different for different swelling degree. Another possibility to compare the outcomes is to compare them at the same output volume as shown in Fig. 10(c) and (d). It can still be seen that swelling enhances the strength at both high and low Peclet numbers in some volume regimes. The curves in both (c) and (d) always tend to converge in the long run, because eventually all the contents will be extracted. However, in the regime of intermediate volume, the strength is significantly enhanced by swelling. Therefore, how large is the effect on the strength depends on how much fluid passes through the porous medium.

Let’s consider again a single filter basket with 7g of coffee powder inside; if the bulk density is 400kg/m$^3$, the volume of the coffee bed will be 17.5ml. Therefore when 25ml of water is pushed through, the volume of the final liquid in the cup normalised by the volume of the coffee bed is $Q_{acc}/V_{bed}$ is 1.43, which falls to a regime where the effect of swelling is quite large in Fig. 10(c). As for low Peclet numbers, it only happens in some clogged regions of the coffee bed, and it is difficult to estimate the actual fluid volume through these regions. However, since the final outcome is dominated by the
FIG. 12: Strength of the extraction of a porous medium. For the solid lines: $H_e$ is fixed, for the dash lines $H_e$ is varying according to Eq. (19). (a) $Pe = 18.23$. (b) $Pe = 0.44$. 

high Peclet number regions, it is safe to conclude that a small degree of swelling will enhance the strength considerably.

C. Results considering the varying geometric hindrance

The single grain simulations are performed again with the same settings as in Fig. 6 but with the geometric hindrance factor varying according to Eq. (19). The results are shown in Fig. 11. As can be seen from Fig. 11, swelling barely has effects on the extraction at both $Pe = \infty$ and $Pe = 0$. The explanation for this is that, swelling increases the volume of the grain and also increases the diffusion coefficient. The increase of volume impedes the extraction while the increase of the diffusion coefficient enhances it. The impediment and the enhancement cancel each other, leading to a trivial combined effect on the extraction. Porous medium simulations are also performed. The two cases studied above are rerun using Eq. (19). The evolutions of the strength against the normalised time are shown in Fig. 12. The solid lines are from the previous simulations with $H_e$ fixed, the dash lines $H_e$ are the new results with $H_e$ varying according to Eq. (19). As can be seen, the inclusion of the effects of varying $H_e$ only slightly enhances the strength. The larger the swelling degree the larger the enhancement, but the enhancement is always very small.

IV. SUMMARY AND CONCLUSIONS

In this article, we propose a swelling model that can consider the influences of swelling on both intra-grain and inter-grain transport. The model is used to investigate how a small particle swelling (< 8%) affects the extraction of coffee. Swelling affects the extraction through two ways: it changes the diffusion of compounds inside the grains, and it also changes the flow around the grains. Our results show that the effect of the altered diffusion inside the grain is very small and almost negligible, while the effect of the altered flow around the grains is more significant. At high Peclet numbers, where normal brewing processes operate, even though the extraction rate is only slightly decreased by swelling, the strength is considerably increased at both fixed brewing time and fixed brewing fluid volume. In our simulation, the increase of strength can be as large as 40% at fixed brewing time (at $tD^*/\bar{R}^2 \approx 0.2$), and 12% at fixed brewing fluid volume (at $Q_{acc}/V_{bed} \approx 1.43$). If the Peclet number is very small, the influence of swelling on the extraction rate is significant, but its influence on the strength is only significant in certain parameter regimes. At fixed brewing time, the effect of swelling on the strength is only important when the brewing time is much larger than the swelling time (i.e. typical diffusive time since $T_s \approx T_d$). At fixed brewing volumes, the effect of swelling on the strength is significant when a small volume ($Q_{acc}/V_{bed} < 0.4$) of fluid is flowed through the bed. In reality, the brewing outcome is dominated by the high Peclet number regions. Our results indicate that a small swelling degree will still considerably enhance the filtered coffee strength at both fixed brewing time and fixed brewing fluid volume. Since the perception of the compounds in mouth is a very nonlinear process, a minor change on the strength could lead to very different taste.

In principle, a barista could intensify or alleviate the effect of swelling by decreasing or increasing the headspace above the coffee cake in the extraction chamber. A barista could also use water with a specific chemistry, or use the pre-infusion process to facilitate swelling. Therefore, swelling has the potential to be an independent variable that can be controlled to produce an ideal espresso, although in most cases, it is a dependent variable determined at the same time by the roasting degree, the particle size, and the temperature.

ACKNOWLEDGEMENT

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DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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