Supplementary materials: A multiscale model for espresso brewing: asymptotic analysis and numerical simulation

Y. Grudeva¹, K. Moroney^{2,3}, and J. M. Foster^{1,4}

¹School of Mathematics and Physics, University of Portsmouth, Lion Terrace, PO1 3HF, UK

²Mathematics Applications Consortium for Science and Industry (MACSI), Department of Mathematics and Statistics, University of Limerick, Limerick V94

T9PX, Ireland

³SSPC, The SFI Research Centre for Pharmaceuticals, University of Limerick, Limerick, V94T9PX, Ireland

⁴The Faraday Institution, Quad One, Becquerel Avenue, Harwell Campus, Didcot, OX11 0RA, UK

A Liquid flow for a fixed pressure device

Darcy's law is normally applied to systems where the porous medium is fully saturated by the fluid, however, assuming that the infiltration in the pores is instantaneous allows us to use Darcy's Law without taking into account the change in hydraulic conductivity to determining the flux during the wetting process. The flow problem is given by

$$q^* = -\frac{\kappa^*}{\mu^*} \frac{\partial P^*}{\partial z^*}$$
 and $\frac{\partial q^*}{\partial z^*} = 0,$ (A1)

where P^* is the liquid overpressure, κ^* is the permeability of the packed bed and μ^* is the liquid viscosity. The pressure at the inlet is specified by the pump. Due to the infiltrating liquid being considerably more viscid than the air being displaced by it, we apply a zero overpressure condition on the wetting interface at $z^* = s_w^*(t^*)$, giving

$$P^*|_{z^*=0} = P^*_{app}$$
 and $P^*|_{z^*=s^*_w(t^*)} = 0$ for $t^* < t^*_w$, (A2)

The same condition for overpressure will be applied at the outlet $z^* = L^*$ after the system is fully wet,

$$P^*|_{z^*=L^*} = 0 \quad \text{for} \quad t^* > t^*_w.$$
(A3)

From here, it's straightforward to solve (A1)-(A3) for the flux q^* and the position of the wetting front s_w^* .

B Coffee conservation at the wetting front

As the water front advances into the bed, a fraction of the coffee solubles is moved from the liquid into the pore space inside boulders and will remain there until dissolution begins. The total space within boulders per unit volume of bed that can be infiltrated by liquid is given by

$$\phi_b \varphi_{lb} = n_b \frac{4}{3} \pi R_0^{*3} \varphi_{lb}, \tag{B1}$$

where n_b is the number density of boulders. Consequently, we write the volume of space in all boulders that is being swept by the moving front per unit time in a cross-sectional area A of the bed located at the wetting interface,

$$A\frac{ds_{w}^{*}}{dt^{*}}n_{b}\frac{4}{3}\pi R_{0}^{*3}\varphi_{lb}.$$
(B2)

This space is filled with liquid carrying solubles at a concentration c_l . To account for the loss of these solubles that infiltrate the pore space within the boulders local to the front, we define a sink term at the front:

$$G_{bw}^* = \delta(z^* - s_w^*) \frac{ds_w^*}{dt^*} c_l^* \phi_b \varphi_{lb}, \tag{B3}$$

where $\delta(\eta)$ is the Dirac delta function localised at the front. We define η to be the distance from the water front, given by

$$\eta = z^* - s_w^*. \tag{B4}$$

We modify (9) local to the front using the sink term, giving

$$-\phi_l \frac{ds_w^*}{dt^*} \frac{\partial c_l^*}{\partial \eta} + \phi_l \frac{\partial c_l^*}{\partial t} + \frac{\partial \mathcal{F}_l^*}{\partial \eta} = b_b^* G_b^* + b_f^* G_f^* - G_{bw}^*.$$
(B5)

Let $\epsilon \ll 1$ and the region $[-\epsilon, +\epsilon]$ extends just barely around the interface at $\eta = 0$ in each direction. Applying the variable change (B4) and integrating (B5) over this region gives

$$\int_{-\epsilon}^{\epsilon} -\phi_l \frac{ds_w^*}{dt^*} \frac{\partial c_l^*}{\partial \eta} + \phi_l \frac{\partial c_l^*}{\partial t} + \frac{\partial \mathcal{F}_l^*}{\partial \eta} d\eta = \int_{-\epsilon}^{\epsilon} b_b^* G_b^* + b_f^* G_f^* - G_{bw}^* d\eta.$$
(B6)

Taking the limit of thickness $\epsilon \to 0$ and evaluating the integrals gives

$$-\frac{ds_w^*}{dt^*}\phi_l c_l^*|_{-\epsilon}^{\epsilon} + \mathcal{F}_l^*|_{-\epsilon}^{\epsilon} = -\frac{ds_w^*}{dt^*}\phi_b\varphi_{lb}c_l^*|_{\eta=0}.$$
 (B7)

Since c_l^* does not exist below the interface at $\eta > 0$ and as $\epsilon \to 0$ we can approximate all positions local to the front to be at $\eta = -\epsilon$, allowing an infinitely small error of size ϵ , we can write (B7) as

$$-\frac{ds_w^*}{dt^*}\phi_l c_l^*|_{z^*=s_w(t)} + \mathcal{F}_l^*|_{z^*=s_w^*(t^*)} = \frac{ds_w^*}{dt^*}\phi_b\varphi_{lb}c_l^*|_{z=s_w^*(t^*)}.$$
 (B8)

C Diffusion from boulders - Diffusion in a sphere with a time-dependent boundary condition

In this section, we relate the concentration $c_{l,0}^{(i)}$ at the surface of the boulders and the flux $\mathcal{F}_{b,0}^{(i)}$ across their surface. We solve the boulder equations given in the main paper (68)–(69) for each position $z = z_0$, $0 < z_0 < 1$ where $z_0 = s_d^-(t_0)$. The initial condition is defined at t_0 where $z_0 = s_d^-(t_0)$, by $c_{b,0}^{(i)}(s_d^-(t_0), r_b, t_0)$ and needs to be determined by matching into region (ii). The surface concentration $c_{l,0}^{(i)}(z_0, t)$ is assumed known but needs to be determined as a solution to (73) from the main paper. Thus the problem reduces to

$$\frac{\partial c_{b,0}^{(i)}}{\partial t} = \frac{1}{r_b^2} \frac{\partial}{\partial r_b} \left(r_b^2 D_{sb} \frac{\partial c_{b,0}^{(i)}}{\partial r_b} \right),\tag{C1}$$

$$-D_{sb}\frac{\partial c_{b,0}^{(1)}}{\partial r_b}\Big|_{r_b=0} = 0, \quad c_{b,0}^{(1)}|_{r_b=1} = c_{l,0}^{(1)}(z_0, t).$$
(C2)

$$c_{b,0}^{(i)}(s_d^-(t_0), r_b, t_0) = \hat{c}_b(t_0), \tag{C3}$$

where $\hat{c}_b(t_0)$ denotes the radially uniform concentration in the boulders exiting region (ii). The aim here is to solve for $c_{b,0}^{(i)}(z_0, r_b, t, c_{l,0}^{(i)}(z_0, t))$, to evaluate the flux through the surface $\mathcal{F}_{b,0}^{(i)}(z_0, 1, t, c_{l,0}^{(i)}(z_0, t)) = -D_{sb} \frac{\partial c_{b,0}^{(i)}}{\partial r_b}\Big|_{r_b=1}$ and hence find $G_{b,0}^{(i)} = \mathcal{F}_{b,0}^{(i)}\Big|_{r_b=1}/Q_b$ and substitute into (67) in the main paper. To solve equations (C1)–(C3) the following substitution is made

$$c_{b,0}^{(i)} = \frac{w}{r_b},\tag{C4}$$

which reduces the diffusion equation to

$$\frac{\partial w}{\partial t} = D_{sb} \frac{\partial^2 w}{\partial r_b^2},\tag{C5}$$

with boundary conditions

$$w|_{r_b=0} = r_b c_{b,0}^{(i)}|_{r_b=0} = 0, \quad w|_{r_b=1} = r_b c_{b,0}^{(i)}|_{r_b=1} = c_{l,0}^{(i)}(z_0,t) = f(t).$$
 (C6)

and initial condition

$$w|_{t=t_0} = r_b \hat{c_b}(t_0).$$
 (C7)

Let

$$w(r_b, \tilde{t}) = u(r_b, \tilde{t}) + v(r_b, \tilde{t}), \quad \text{and} \quad t = t_0 + \tilde{t}$$
(C8)

where

$$u(r_b, \tilde{t}) = r_b \tilde{f}(\tilde{t}), \qquad u|_{r_b=0} = 0, \qquad u|_{r_b=1} = \tilde{f}(\tilde{t}),$$
 (C9)

where $\tilde{f}(\tilde{t}) = f(\tilde{t} + t_0)$. Then (C5) becomes the following BVP for $v(r_b, \tilde{t})$:

$$\frac{\partial v}{\partial \tilde{t}} = D_{sb} \frac{\partial^2 v}{\partial r_b^2} - \frac{\partial u}{\partial \tilde{t}}, \qquad \qquad \frac{\partial u}{\partial \tilde{t}} = r_b \dot{\tilde{f}}(\tilde{t}) \tag{C10}$$

with boundary conditions

$$v|_{r_b=0} = 0,$$
 $v|_{r_b=1} = 0,$ (C11)

and initial condition

$$v|_{\tilde{t}=0} = r_b \hat{c}_b(t_0) - u|_{\tilde{t}=0}.$$
 (C12)

Now $v(r_b, \tilde{t})$ can be found using an eigenfunction expansion. The eigenvalues and eigenfunctions are

$$\lambda_n = n\pi$$
, for $n = 1, 2, \dots$ $S_n(r_b) = \sin(\lambda_n r_b)$. (C13)

Let

$$S(r_b, \tilde{t}) = -\frac{\partial u}{\partial \tilde{t}} = -r_b \dot{\tilde{f}}(\tilde{t})$$
(C14)
 ∞

$$=\sum_{n=1}^{\infty}\hat{S}_n(\tilde{t})\sin(\lambda_n r_b),\tag{C15}$$

and

$$v(r_b, \tilde{t}) = \sum_{n=1}^{\infty} \hat{v}_n(\tilde{t}) \sin(\lambda_n r_b), \qquad (C16)$$

where $\hat{S}_n(\tilde{t})$ and $\hat{v}_n(\tilde{t})$ are the coefficients for the respective Fourier series. Then

$$\frac{\partial v}{\partial \tilde{t}} = \sum_{n=1}^{\infty} \dot{v_n} \sin(\lambda_n r_b), \tag{C17}$$

$$\frac{\partial^2 v}{\partial r_b^2} = \sum_{n=1}^{\infty} \hat{v_n}(\tilde{t})(-\lambda_n^2) \sin(\lambda_n r_b).$$
(C18)

Substituting these expansions back in (C10),

$$\frac{\partial v}{\partial \tilde{t}} - D_{sb} \frac{\partial^2 v}{\partial r_b^2} - S(r_b, \tilde{t}) = 0, \qquad (C19)$$

and thus the following must be true for all values of n:

$$\sum_{n=1}^{\infty} \left(\dot{\hat{v}_n} + D_{sb} \lambda_n^2 \hat{v}_n - \hat{S}_n(\tilde{t}) \right) \sin(\lambda_n r_b) = 0, \qquad (C20)$$

giving a system of ODEs for $\hat{v_n}(r_b, \tilde{t})$:

$$\frac{d\hat{v_n}}{d\tilde{t}} + D_{sb}\lambda_n^2\hat{v_n} = \hat{S_n}(\tilde{t}),\tag{C21}$$

which we solve with an integrating factor. After multiplying by $e^{D_{sb}\lambda_n^2 \tilde{t}}$ we have

$$\frac{d}{d\tilde{t}} \left(e^{D_{sb}\lambda_n^2 \tilde{t}} \hat{v}_n(\tilde{t}) \right) = e^{D_{sb}\lambda_n^2 \tilde{t}} \hat{S}_n(\tilde{t}).$$
(C22)

Integrating this, we obtain

$$e^{D_{sb}\lambda_n^2 \tilde{t}} \hat{v}_n(\tilde{t}) = \int_0^{\tilde{t}} e^{D_{sb}\lambda_n^2 \tau} \hat{S}_n(\tau) d\tau + A_n, \qquad (C23)$$

which we can write as

$$\hat{v}_{n}(\tilde{t}) = \int_{0}^{t} e^{-D_{sb}\lambda_{n}^{2}(\tilde{t}-\tau)} \hat{S}_{n}(\tau) d\tau + e^{-D_{sb}\lambda_{n}^{2}\tilde{t}} A_{n}.$$
(C24)

Thus,

$$v(r_b, \tilde{t}) = \sum_{n=1}^{\infty} \left(\int_0^{\tilde{t}} e^{-D_{sb}\lambda_n^2(\tilde{t}-\tau)} \hat{S}_n(\tau) d\tau + e^{-D_{sb}\lambda_n^2 \tilde{t}} A_n \right) \sin(\lambda_n r_b).$$
(C25)

The coefficients A_n we obtain from the initial condition:

$$r_b \hat{c}_b(t_0) - u(r_b, 0) = \sum_{n=1}^{\infty} A_n \sin(\lambda_n r_b).$$
 (C26)

This is a Fourier sine series in which

$$A_{n}(\tilde{t}) = 2 \int_{0}^{1} (r_{b}\hat{c}_{b}(t_{0}) - u(r_{b}, 0)) \sin(\lambda_{n}r_{b}) dr$$

$$= 2(\hat{c}_{b}(t_{0}) - c_{l,0}^{(i)}(z_{0}, t_{0})) \frac{(-1)^{n+1}}{n\pi}.$$
 (C27)

The flux at the boulder surface is given by

$$\mathcal{F}_{b,0}^{(i)}\Big|_{r_b=1} = -D_{sb}\frac{\partial c_{b,0}^{(i)}}{\partial r_b}\Big|_{r_b=1} = D_{sb}\left(\frac{w}{r_b^2} - \frac{1}{r_b}\frac{\partial w}{\partial r_b}\right)\Big|_{r_b=1} = D_{sb}\left(w - \frac{\partial w}{\partial r_b}\right)\Big|_{r_b=1}.$$
(C28)

Evaluating at $r_b = 1$ gives

$$\mathcal{F}_{b,0}^{(i)}\Big|_{r_b=1} = D_{sb}\left(\tilde{f}(\tilde{t}) + \sum_{n=1}^{\infty} \hat{v_n}(\tilde{t}) \sin n\pi\right)$$

$$-D_{sb}\left(\tilde{f}(\tilde{t}) + \sum_{n=1}^{\infty} \hat{v_n}(\tilde{t})n\pi \cos n\pi\right)$$
$$= -D_{sb}\sum_{n=1}^{\infty} n\pi (-1)^n \hat{v_n}(\tilde{t}), \qquad (C29)$$

where $\sin n\pi = 0$ and $\cos n\pi = -1^n$ have been used. The expression for $\hat{v}_n(\tilde{t})$ is known in terms of $S_n(\tilde{t})$, so it remains to calculate $S_n(\tilde{t})$. We get and

$$\hat{S}_{n}(\tilde{t}) = 2 \int_{0}^{1} -r_{b}\dot{\tilde{f}}(\tilde{t})\sin(\lambda_{n}r_{b})dr_{b} = -2\dot{c}_{l,0}^{(i)}(\tilde{t})\frac{(-1)^{n+1}}{n\pi}.$$
(C30)

Then combining equations (C29), (C24), (C27) and (C30) gives

$$\mathcal{F}_{b,0}^{(i)}\Big|_{r_b=1} = 2D_{sb} \sum_{n=1}^{\infty} e^{-n^2 \pi^2 D_{sb} \tilde{t}} \\ \times \left(c_{\hat{b}0}(t_0) - c_{l,0}^{(i)}(z_0, t_0) - \int_0^{\tilde{t}} \dot{\tilde{f}}(\tau) e^{n^2 \pi^2 D_{sb} \tau} \mathrm{d}\tau \right).$$
(C31)

Thus, we write down the solution

$$w(r_b, \tilde{t}) = r_b \tilde{f}(\tilde{t})$$
$$+ \sum_{n=1}^{\infty} \left(\int_{t_0}^{\tilde{t}} e^{-D_{sb}\lambda_n^2(\tilde{t}-\tau)} \hat{S}_n(\tau) d\tau + e^{-D_{sb}\lambda_n^2 \tilde{t}} A_n \right) \sin(\lambda_n r_b). \tag{C32}$$

Finally, we reverse the substitution (C4):

$$c_{b,0}^{(i)} = c_{l,0}^{(i)}(z_0, t) + \frac{2}{r_b} \sum_{n=1}^{\infty} \left(\frac{(-1)^{n+1}}{n\pi} \right) e^{-D_{sb}n^2\pi^2(t-t_0)} \left(\hat{c}_b(t_0) - c_{l,0}^{(i)}(z_0, t_0) - \int_{t_0}^t e^{D_{sb}n^2\pi^2\tau} \dot{c}_{l,0}^{(i)}(\tau) d\tau \right) \sin n\pi r_b.$$
(C33)

In summary, the flux at the boulder surface required for equation (67) in the main paper is given by

$$\mathcal{F}_{b,0}^{(i)}(z_0, 1, t, c_{l,0}^{(i)}(z_0, t)) = 2D_{sb} \sum_{n=1}^{\infty} e^{-n^2 \pi^2 D_{sb}(t-t_0)} \left(c_{b,0}^{(i)}(s_d^-(t_0), 1, t_0) - c_{l,0}^{(i)}(z_0, t_0) - \int_{t_0}^t c_{i,0}^{(i)}(z_0, \tau) e^{n^2 \pi^2 D_{sb} \tau} \mathrm{d}\tau \right).$$
(C34)

D Asymptotic analysis for unsaturation extraction

Here we present the modified structure of the asymptotically reduced model in the case where a saturated region does not form, see §2.7 in the main paper. Here, we maintain regions (i) and (ii), however, region (ii) is studied under the change of variables

$$\epsilon w = z - s_w,\tag{D1}$$

which replaces (40) in the main paper, and $w \in (-\infty, 0)$. We emphasize that in the case of no-saturation the saturation interface, s_d , does not exist and instead there is a slender layer, region (ii), adjacent to the wetting front s_w in which the concentration in the liquid changes markedly, but not so much as to fully saturate the liquid. The boundary conditions of region (ii) are now as follows:

$$c_{f,0}^{(\mathrm{ii})}|_{w=0} = c_{f,0}, \qquad c_{b,0}^{(\mathrm{ii})}|_{w=0} = c_{b,0} + \varphi_{lb}c_{l,0}|_{w=0}^{(\mathrm{ii})}, \qquad \frac{\partial c_{l,0}^{(\mathrm{ii})}}{\partial w}\Big|_{w=0} = 0.$$
(D2)

The location of region (ii) is given by the wetting front and matching conditions to region (i) given by (47) and (D2) result in the modification of (52) given by

$$\left(-\dot{s_w}\frac{\phi_l}{\phi_T} + q\right) \left(c_{l,0}^{(\text{ii})}|_{w=0} - c_{l,0}^{(\text{i})}|_{z=s_w^-(t)}\right) = \int_{-\infty}^0 G_{f,-1}^{(\text{ii})} dw.$$
(D3)

Performing the same order of operations as in (53) - (56), we integrate the concentration of the fines over region (ii) to arrive at

$$-\dot{s}_{w} \int_{-\infty}^{0} \int_{0}^{1} r_{f}^{2} \frac{\partial c_{f,0}^{(\text{ii})}}{\partial w} dr_{f} dw = \int_{-\infty}^{0} -Q_{f} G_{f,-1}^{(\text{ii})} dw.$$
(D4)

Evaluating the integral on the left-hand side and substituting (D3) to eliminate the integral of the fine dissolution rate, we write down

$$\frac{\dot{s}_w}{3Q_f} \left(c_{f,0} - c_{l,0}^{(i)} |_{z=s_w^-(t)} \right)$$
$$= \left(-\dot{s}_w \frac{\phi_l}{\phi_T} + q \right) \left(c_{l,0}^{(ii)} |_{w=0} - c_{l,0}^{(i)} |_{z=s_w^-(t)} \right). \tag{D5}$$

Following the solution to the diffusion problem in the boulders given in appendix C, gives the mass transfer rate $G_{b,0}^{(i)}$, that is the relationship between $c_{l,0}^{(i)}$ and the soluble concentration in the boulders immediately after wetting the \hat{c}_b , where $\hat{c}_b = c_{b,0} + \varphi_{lb}c_{l,0}|_{w=0}^{(i)}$. The result in (D5) allows us to write the problem in region (i) independently of the concentrations in region (ii) by writing the initial boulder concentration as,

$$c_{b,0}^{(i)}|_{s_{w}^{-}(t)} = c_{b,0} + \varphi_{lb} \left(\frac{\dot{s}_{w} \left(c_{f,0} - c_{l,0}^{(i)}|_{z=s_{w}^{-}(t)} \right)}{3Q_{f} \left(-\dot{s}_{w} \frac{\phi_{l}}{\phi_{T}} + q \right)} + c_{l,0}^{(i)}|_{z=s_{w}^{-}(t)} \right).$$
(D6)

Thus, we write the problem in region (i),

$$\left(\frac{\phi_l}{\phi_T} + \frac{1}{3Q_f}\right)\frac{\partial c_{l,0}^{(i)}}{\partial t} + q\frac{\partial c_{l,0}^{(i)}}{\partial z} = G_{b,0}(c_{l,0}^{(i)}) \quad \text{with} \quad c_{l,0}^{(i)}|_{z=0} = 0, \tag{D7}$$

and use (D5) to find the solution $c_{l,0}^{(\text{ii})}$ at the front.

E Numerical Methods

In this section, we discuss the numerical schemes and their implementation used to solve the full (23)-(28) and reduced model (74) and (75). Section §E.1 presents the former and §E.2 the latter.

E.1 Full model

Solution of the full model requires numerical treatment of the system (23)-(29) given in the main paper. The equations in the liquid, i.e., those containing partial derivatives in the macroscopic coordinate z, are discretised in space using a second order finite element (FE) scheme. The equations in the grains, i.e., those containing partial derivatives in r, are discretised in space using a second order control volume (CV) method.

After applying these spatial discretisations the system of coupled PDEs is converted into a large system of coupled differential-algebraic equations (DAE) which can readily be handed to any number of numerical integrators. In our case we chose to use MATLAB[®]'s solver ode15s which uses adaptive time stepping. We choose this because during infiltration, the wet region is expanding with time causing a time-dependent domain defined by the position of the boundary $z = s_w(t)$. The moving domain is mapped to a static domain defined by the current position of the wetting interface and by definition in the dry region we have $c_l = 0$, $c_f = c_{f,init}$ and $c_b = c_{b,init}$. In this sense, our approach is similar to the so-called "method of lines", albeit a multiscale domain.

E.1.1 Numerical discretisation in the liquid - FE

The transport problem in the liquid is given by (23). To reiterate, we have

$$\frac{\phi_l}{\phi_T}\frac{\partial c_l}{\partial t} + \frac{\partial \mathcal{F}_l}{\partial z} = G_f + G_b, \quad \mathcal{F}_l = -D_{\text{eff}}\frac{\partial c_l}{\partial z} + qc_l, \quad (E1)$$

with
$$c_l|_{z=0} = 0$$
 and
$$\begin{cases} -\dot{s}_w c_l + \mathcal{F}_l \Big|_{z=s_w(t)} = 0 \quad \text{for} \quad 0 < t < 1, \\ \frac{\partial c_l}{\partial z} \Big|_{z=1} = 0 \quad \text{for} \quad t \ge 1. \end{cases}$$
 (E2)

During the wetting phase, the domain in which we seek a solution for the concentrations of solubles c_l , c_f and c_b expands with the front. Before the coffee bed is completely wet at t = 1, c_l is defined for $z \in (0, s_w)$. To avoid solving in a time-dependent spatial domain, we introduce the following transformation:

$$t = \tau, \qquad \eta = \frac{z}{s_w(t)},\tag{E3}$$

such that $\eta \in (0, 1)$ and

$$\frac{\partial}{\partial z} = \frac{1}{s_w} \frac{\partial}{\partial \eta}, \quad \text{and} \quad \frac{\partial}{\partial t} = -\eta \frac{\dot{s_w}}{s_w} \frac{\partial}{\partial \eta} + \frac{\partial}{\partial \tau}.$$
 (E4)

From here, we will maintain using the variable t for the simplicity of the notation. Under the transformation (E3), the problem in the liquid (23)-(29) becomes

$$\frac{\phi_l}{\phi_T}\frac{\partial c_l}{\partial t} - \frac{\phi_l}{\phi_T}\eta\frac{\dot{s_w}}{s_w}\frac{\partial c_l}{\partial \eta} = \frac{D_{eff}}{s_w^2}\frac{\partial^2 c_l}{\partial \eta^2} - \frac{q}{s_w}\frac{\partial c_l}{\partial \eta} + G_b + G_f.$$
(E5)

The boundary conditions supplementing (E5) are derived from (E2) transformed onto η coordinate:

$$c_l|_{\eta=0} = 0, \quad \text{and} \quad \frac{\partial c_l}{\partial \eta}\Big|_{\eta=1} = 0,$$
 (E6)

where, upon applying the transformation (E3), the two cases of the boundary condition (E2b) both collapse to (E6b). The initial condition is given by

$$c_l|_{t=0} = 0.$$
 (E7)

We begin by discretising the η -domain in η into N + 1 equally spaced grid points η_i for i = 1, ..., N + 1. The width of the intervals between neighbouring points is denoted by Δ . We also introduce N half-points denoted by $\eta_{i+1/2} = \frac{1}{2}(\eta_i + \eta_{i+1})$ for i = 1, ..., N. From now on, we will drop the subscript l in order to simplify the notation and note that in this subsection c will refer to concentration in the liquid. We denote the values of c by c_i for i = 1, ..., N + 1 at the grid points. The spatial derivatives in (E5) are discretised using a finite element scheme. Following the frequently used technique, we approximate the concentration in the liquid as a linear combination of piecewise linear basis functions, also referred to as "hat" functions. For the dependent variable $c(\eta, t)$ we write

$$c = \sum_{i} c_{i}(t)\psi_{i}(\eta) \quad \text{where} \quad \psi_{i}(\eta) = \begin{cases} \frac{\eta - \eta_{i-1}}{\eta_{i} - \eta_{i-1}} & \text{for} \quad \eta_{i-1} \le \eta \le \eta_{i} \\ \frac{\eta_{i+1} - \eta_{i}}{\eta_{i+1} - \eta_{i}} & \text{for} \quad \eta_{i} \le \eta \le \eta_{i+1} \\ 0 & \text{otherwise}, \end{cases}$$
(E8)

in which the denominators in the definition of the basis functions $\psi_i(\eta)$ in the right-hand side of (E8) could be further simplified when choosing a uniform grid with $\eta_{i+1} - \eta_i = \Delta, \forall i \in 1, ..., N + 1$.

Our aim is to derive a system of spatially discretised equations from (E5). This is done so by substituting the form (E8) into (E5), multiplying through by each of the test functions $\psi_j(\eta)$ for j = 1, ..., N + 1 and integrating over the domain $\eta \in (0, 1)$. Upon denoting the time derivatives $\dot{c}_i = \frac{dc_i}{dt}$, we arrive at

$$\frac{\phi_l}{\phi_T} \sum_i \dot{c}_i \int_0^1 \psi_i \psi_j d\eta = \sum_i \left(c_i \frac{\phi_l}{\phi_T} \frac{\dot{s}_w}{s_w} \int_0^1 \eta \psi_i' \psi_j d\eta - D_{\text{eff}} \frac{c_i}{s^2} \int_0^1 \psi_i' \psi_j' d\eta - q \frac{c_i}{s_w} \int_0^1 \psi_i' \psi_j d\eta + \int_0^1 (G_b + G_f) \psi_j d\eta \right).$$
(E9)

The integrals in (E9) that contain only the basis functions and/or their derivatives often appear in FE schemes and they can be computed exactly.

The final two terms in (E9) are a linear functions of c_i due to our choice of a mass transfer function. In the future, we hope to gain a more complete perspective of the dynamics of solubles and their transport through the surface of the grains and be able to adjust the functional form of the mass transfer without significantly changing the numerical scheme. To perform the integration independent of our choice of a mass transfer rate, we approximate the dependent variable c_i in the integrand as a piecewise constant over each interval between grid points. The error introduced by this approximation is $O(\Delta^2)$ and is comparable to the error incurred by the approximation in (E8) and consequentially it will not decrease the accuracy of the scheme. The value of the concentration c_i over the interval (η_i, η_{i+1}) is approximated as the value it takes at the midpoint of the corresponding interval, $\eta_{i+1/2}$. This gives

$$G = G_{b,i+1/2} + G_{f,i+1/2} = \frac{G_{f,i} + G_{f,i+1}}{2} + \frac{G_{f,i} + G_{f,i+1}}{2},$$
 (E10)

where we introduce G to be the sum of the extraction terms for easier notation.

Upon evaluating the the integrals in (E9), we write the full discretised system of equations to be solved in the liquid by substituting j = 1, ..., N + 1 in (E9) and evaluating the sum. The boundary conditions (E6) are imposed as follows:

$$c_1 = 0, \qquad \frac{c_{N+1} - c_N}{\Delta} = 0.$$
 (E11)

At j = 1:

$$c_1 = 0. \tag{E12}$$

At j = 2, ..., N:

$$\frac{\phi_l}{\phi_T} \left(c_{i-1} \frac{\Delta}{6} + \dot{c}_i \frac{2\Delta}{3} + c_{i+1} \frac{\Delta}{6} \right) = \frac{\phi_l}{2\phi_T} \frac{\dot{s}_w}{s_w} \left(\eta_{j-\frac{1}{3}} (c_i - c_{i-1}) + \eta_{j+\frac{1}{3}} (c_{i+1} - c_i) \right) \\
+ \frac{D_{\text{eff}}}{s_w^2} \left(\frac{c_{i-1} - 2c_i + c_{i+1}}{\Delta} \right) \\
- \frac{q}{s_w} \left(\frac{c_{i+1} - c_{i-1}}{2} \right) + \Delta \frac{G_{i-\frac{1}{2}} + G_{i+\frac{1}{2}}}{2}.$$
(E13)

At j = N + 1:

$$\frac{\phi_l}{\phi_T} \left(c_{N+1} \frac{\Delta}{3} + c_N \frac{\Delta}{6} \right) = \frac{\phi_l}{6\phi_T} \frac{\dot{s}_w}{s_w} \left(-c_N (2\eta_{N+1} + \eta_N) + c_N (2\eta_{N+1} + \eta_N) \right)
- \frac{q}{s_w} c_{N+1} + \frac{D_{\text{eff}}}{s_w^2} \left(\frac{c_N - c_{N+1}}{\Delta} \right)
+ \frac{q}{s_w} \left(\frac{c_{N+1} + c_N}{2} \right) + \frac{\Delta}{2} G_{N+\frac{1}{2}}.$$
(E14)

Imposing the boundary condition (E11) introduces an algebraic equation to a system of ODEs. This DAE system is written in matrix form $\mathcal{M}\mathbf{c} = f(\mathbf{c})$ and implemented in MATLAB[®]'s solver ode15s.

E.1.2 Numerical discretisation in the grains - CV

The dimensionless equations for the coffee grains (25)-(26), repeated here, are

$$\frac{\partial c_k}{\partial t} + \frac{1}{r_k^2} \frac{\partial}{\partial r_k} \left(r_k^2 \mathcal{F}_k \right) = 0, \quad \mathcal{F}_k = -D_{sk} \frac{\partial c_k}{\partial r_k}, \tag{E15}$$

with
$$\mathcal{F}_k\Big|_{r_k=0} = 0$$
 and $\mathcal{F}_k\Big|_{r_k=1} = Q_k G_k.$ (E16)

for k = b, f for boulders and fines respectively. The initial condition for the fines is

$$c_f|_{t=0} = c_{f,\text{init}}.\tag{E17}$$

The surface fluxes (27) are given by

$$G_{k} = \frac{b_{k}}{\epsilon} \begin{cases} 0 & \text{if } z > s_{w}(t) \\ 1 - c_{l} & \text{if } c_{k}|_{r_{k}=1} \ge 1 \\ c_{k}|_{r_{k}=1} - c_{l} & \text{if } c_{k}|_{r_{k}=1} < 1 \end{cases}$$
(E18)

The condition for the boulders at the front (28) is given by

$$c_b|_{t=s_w^{-1}(z)} = c_{b,\text{init}} + c_l|_{t=s_w^{-1}(z)}\varphi_{lb}.$$
(E19)

In order to impose the initial condition in the boulders as the front passes and fills them with liquid at a concentration c_l we would require a boundary condition that depends on the solution at the last step. The built-in solver does not have these options but an alternative would be to assume saturation and impose a condition on boulders being filled up at saturation concentration immediately after wetting. To avoid the complication or inaccuracy that this would pose to the implementation of these numerical schemes, we apply $\varphi_{lb} = 0$. This may not be a realistic value for this parameter, however for the purpose of comparing asymptotic solutions and solutions to the full model, it is not crucial for parameter values to be completely physical. An alternative suggestion would be to assume saturation and impose $c_b|_{z=s_w(t)} = c_{b,\text{init}} + c_{\text{sat}}\varphi_{lb}$.

We discretise the radial coordinate r_k into M + 1 equally spaced points r_i for i = 1, ..., M + 1 and denote the distance between any two neighbouring points Δr and the concentration of solubles in the grain c_i at the grid points, where i indicates the index of the grid point, not to be confused with the earlier notation for grain species. The problem in both grain types is solved in the same manner, therefore we write down the generalised solution by omitting the species specific parameters. We thus write (E15) as

$$r^{2}\frac{\partial c}{\partial t} = \frac{\partial}{\partial r} \Big(Dr^{2}\frac{\partial c}{\partial r} \Big). \tag{E20}$$

Applying the procedure derived by Zeng et al. [2], we obtain the discretised equations in the grains as follows.

At i = 1

$$\frac{3}{4}V_1\dot{c}_1 + \frac{1}{8}V_2\dot{c}_2 = 0.$$
 (E21)

At
$$i = 2$$

$$\frac{1}{4}V_{1}\dot{c_{1}} + \frac{6}{8}V_{2}\dot{c_{2}} + \frac{1}{8}V_{3}\dot{c_{3}}$$

$$= 4\pi Dr_{5/2}^{2}\frac{c_{3} - c_{2}}{\Delta r} - 4\pi Dr_{3/2}^{2}\frac{c_{2} - c_{1}}{\Delta r}.$$
(E22)
At $i = 2, ..., M$

$$\frac{\frac{1}{8}V_{i-1}\dot{c_{i-1}} + \frac{6}{8}V_i\dot{c}_i + \frac{1}{8}V_{i+1}\dot{c_{i+1}} = 4\pi Dr_{i+1/2}^2\frac{c_{i+1} - c_i}{\Delta r} - 4\pi Dr_{i-1/2}^2\frac{c_i - c_{i-1}}{\Delta r}.$$
(E23)

At
$$i = M$$

$$\frac{1}{8}V_{M-1}c_{M-1} + \frac{6}{8}V_Mc_M + \frac{1}{4}V_{M+1}c_{M+1}$$

$$= 4\pi Dr_{M+1/2}^2 \frac{c_{M+1} - c_M}{\Delta r} - 4\pi Dr_{M-1/2}^2 \frac{c_M - c_{M-1}}{\Delta r}.$$
(E24)
At $i = M + 1$

$$\frac{1}{8}V_M \dot{c_M} + \frac{3}{4}V_{M+1} \dot{c_{M+1}} = -4\pi r_{M+1}^2 QG_{M+1} - 4\pi Dr_{M+1/2}^2 \frac{c_{M+1} - c_M}{\Delta r}.$$
(E25)

Similarly to the problem in the liquid, equations (E11)-(E14) are written in matrix form and coupled to the problem in the liquid when implemented in MATLAB[®].

E.1.3 Coupling the problems

The model could sensibly be described as 1+1D, meaning that the spatial dimensions are almost entirely independent, coupled only by the extraction rates. We design a grid in (z, r), such that at each point in z, denoted by z_i , sits an orthogonal grid for one representative fine and one boulder. At each grid point in z_i we seek a solution for the concentrations of solubles in the liquid at each point and the corresponding concentration profiles across the radii of the fines and boulders. The diffusion problem in the grains is easier to solve numerically as it is not stiff and the concentration gradients are strictly non-negative and therefore it converges numerically for a much smaller number of grid points than the problem in the liquid. Choosing the sparsity of the grids in z and r is crucial because refining the grid spacing in r is computationally expensive.

We seek the solution of the concentration in the liquid $c_l(\eta, t)$ on the transformed grid defined by (E3), and the solution in the grains $c_f(z, r_f, t) c_b(z, r_b, t)$. We always discretise η in the same number of points, however the grid spacing between points in η when projected onto z would increase as the front advances. Advancing the front in time in this manner guarantees that it will land at a grid point in η at each time step and during the initial stages of infiltration, we expect to see rapid increase in the concentration in the liquid in the newly wetted region which needs to be resolved on a large number of points. The difference in the coordinate systems is handled by interpolating the source terms G_f and G_b at each step by doing the following:

- 1. Find the vector of surface concentrations of the grains at the current position of the front and in the entire wet region given by $(0, s_w)$;
- 2. Interpolate the surface concentrations onto $\eta = (0, 1)$ coordinates by "stretching out" the vector on the same number of grid points N + 1 as is η ;
- 3. Evaluate the extraction terms (in η) according to (27) and substitute in (E11)-(E14) to couple to the concentration in the liquid and;
- 4. Interpolate the extraction terms back onto z coordinates to couple the system to the grains (E21)-(E25) in the wet region while all grains in the dry region remain idle.

This procedure allows us to have high resolution of the solution in the wet region and save computational time in stepping forward grains that are in the dry region. We use linear interpolation and the error introduced by this step is consistent with the FE spatial discretisation and using a higher order interpolation method is redundant since the variables have already been approximated as linear functions in the sub-intervals.

E.2 Reduced model

Here we present the first order discretisation of the reduced model in region (i) that leads to a system of linear equations implemented and solved for in Python and the solver is available online at GitHub [1]. As described in §4.5 of the main paper, the asymptotically reduced model requires a coupled PDE and an ODE to be solved, namely (74) and (67) given in the main paper. The former is an ODE that predicts the position of the saturation interface and the latter, a PDE for the evolution of the concentration in the liquid in region (i). The two are coupled by the boulder diffusion problem (68)-(70) and we will need to solve (74) many times to obtain a full picture of the solution in region (i). Since it is only necessary to evaluate the solution in region (i), we will drop the superscript (i) for an easier notation.

The numerical solver is based on a finite difference spatial discretisation and a forward Euler-based method in time for the microscopic equations (68)-(70) and a backward Euler method with upwind approximations of the spatial derivatives for the macroscopic equation (67) and a forward Euler method for determining the location of the saturation interface (74). The two scales are combined by defining a system of the microscale equations at each grid point in the macroscale grid. We note that the analytical solution to the diffusion problem in the boulders is directly available from the analytical solution (71), however a numerical solution is easier to implement in the computational solution as it does not require summation of the series. Overall, as a forward Euler method, the scheme exhibits first-order accuracy.

E.2.1 Numerical discretisation in the liquid

As the saturation front s_d advances down the bed, the spatial domain of region (i) expands so that $z \in [0, s_d(t)]$ until the front reaches the outlet, thereafter the domain remains $z \in [0, 1]$ for the remainder of the brew time. To deal with the expanding domain, we introduce the following variable transform:

$$\eta = \frac{z}{s_d},\tag{E26}$$

such that $z \in [0, s_d]$ and $\eta \in [0, 1]$. Under the transform (E26), we denote the source term on the right-hand side of (67) defined on η coordinates to be \hat{G}_b the problem in the liquid (67) becomes

$$\frac{\partial c_l}{\partial t} = \left(-\frac{q(t)}{\left(\frac{\phi_l}{\phi_T} + \frac{1}{3Q_f}\right)s_d} + \eta \frac{\dot{s_d}}{s_d} \right) \frac{\partial c_l}{\partial \eta} + \frac{\hat{G}_b}{\frac{\phi_l}{\phi_T} + \frac{1}{3Q_f}}, \tag{E27}$$

with initial and boundary conditions derived from (67b)

$$c_l|_{\eta=0} = 0$$
 and $c_l|_{t=0} = 0.$ (E28)

We discretise the time domain into N_t equally-spaced collocation points, such that the intervals separating them are of width Δt , and denoting the points $t = t_i$ for $i = 0, 1, ..., N_t - 1$.¹ The ODE (74) is discretised using a forward Euler method yielding

$$s_d^{i+1} = s_d^i + q^{i+1} \left(\frac{\phi_l}{\phi_T} + \frac{1}{3Q_f} \frac{c_{f,0} - c_l^i |_{z=s_d^i(t)}}{1 - c_l^i |_{z=s_d^i(t)}} \right)^{-1} \Delta t \quad \text{with} \quad s_d^0 = 0,$$
(E29)

allowing us to find the subsequent position of the saturation front given present information.

We now determine the evolution of c_l by discretising the spatial domain $\eta \in (0, 1)$ into N collocation points and denote Δ to be the distance between any two neighbouring points. We denote the values of $c(\eta, t)$ at these points by c_j^{i+1} for j = 0, ..., N - 1, so that the superscript indicates the value of t and the subscript denotes the value of η . We discretise spatial derivatives by a first-order upwind approximation and apply a backward Euler method to evolve the solution in time. This yields the following system to solve for $c_l(\eta, t)$ in the liquid:

$$c_{j}^{i+1} \left(\frac{1}{\Delta t} - \frac{q^{i+1}}{Bs_{d}^{i+1}\Delta} - \frac{\eta_{j}\dot{s_{d}}^{i+1}}{s_{d}^{i+1}\Delta} \right) = \frac{c_{j}^{i}}{\Delta t} - c_{j-1}^{i+1} \left(-\frac{q^{i+1}}{Bs_{d}^{i+1}\Delta} + \frac{\eta_{j}\dot{s_{d}}^{i+1}}{s_{d}^{i+1}}\Delta \right) + \frac{\hat{G}_{j}^{i}}{B},$$
(E30)

with

$$c_0^0 = 0,$$
 (E31)

¹To aid the reader when referring to the code on Github [1], we have adopted different notations in the indexing used the numerical schemes for the full and reduced model. Indexing in the full model starts from i = 1 and for the reduced model from i = 0. We chose this indexing due to the implementation of the full model in MATLAB[®] and the reduced in Python.

where $B = \frac{\phi_l}{\phi_T} + \frac{1}{3Q_f}$ is shortened for compactness.

The spatial domain transformation (E26) and the discretisation of η cause the number of grid points to remain constant but their positions and spacing in the original domain in z will change at each time step. To obtain a solution for the boulder concentration, however, we require a fixed grid in the bed. We discretise z identically to η into N collocation points and denote them by z_j for j = 0, ..., N - 1.

E.2.2 Numerical discretisation in the boulders

The transport of solubles (68)-(70) inside the boulders is solved at each grid point in the bed z_j on a uniform grid in r. We discretise the radial domain into M points, r_k for k = 0, ... M - 1. The problem is essentially radial diffusion in a sphere and we apply a finite-difference approximation. It evolves in time simultaneously with the liquid, and we apply a forward Euler method. The discretised equations for $c_b(z_j, r, t)$ at each z_j are:

$$\frac{c_{b,k}^{i+1} - c_{b,k}^{i}}{\Delta t} = \begin{cases} \frac{D_{sb}}{k\Delta r^{2}} \left((k+1)c_{b,k+1}^{i} - 2kc_{b,k}^{i} + (k+1)c_{b,k-1}^{i} \right), & k \neq 0, M, \\ D_{sb}c_{l}|_{z_{j}}, & k = M, \\ 0, & k = 0. \end{cases}$$
(E32)

The problem in the liquid and the problem in the boulders are coupled by the source term G(z,t) which is given by the flux condition (70)

$$G = -\frac{D_{sb}}{Q_b} \frac{\partial c_b}{\partial r}\Big|_{r=1}.$$
(E33)

Allowing a "time lag" of Δt , we can compute the boulder concentration using concentration in the liquid c_j^{i-1} at the surface from the previous time step. Doing this allows us separate (E30) and (E32) and to solve the boulder diffusion in advance to the liquid transport in order to compute G_j^i directly from the flux condition (E33). The source term is defined on the two macroscopic spatial domains as G(z,t) for the boulders and as $\hat{G}(\eta,t)$ in the liquid. To account for this transformation, at each time step $t = t^i$, we interpolate between the two grids using linear interpolation. The boulders are located at all discrete points z_j , however, only the ones in region (i), i.e. in the domain $z \in (0, s_d^i)$ will be dissolving and there will be no soluble extraction from those outside this region. To account for the different domains, we first identify all points z_j for which $z_j \leq s_d^i$ and we use linear interpolation to "stretch" the values of $G_j \in (0, s_d^i)$ onto $\eta \in (0, 1)$. Now \hat{G}_j^i is used directly in (E30) to obtain the solution in the liquid in $\eta \in (0, 1)$.

References

- GRUDEVA, Y., espresso-model. https://github.com/YoanaGrudeva/ espresso-model, 2020.
- [2] Y. ZENG, P. ALBERTUS, R. KLEIN, N. CHATURVEDI, A. KOJIC, M. Z. BAZANT, AND J. CHRISTENSEN, *Efficient conservative numerical schemes for 1d nonlinear*

spherical diffusion equations with applications in battery modeling, Journal of The Electrochemical Society, 160 (2013), p. A1565.