Code to solve a multiscale model for espresso coffee brewing

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1 Problem formulation

The coffee concentration within the liquid phase, c_l^*, is governed by the following advection-diffusion equation

$$\frac{\partial c_l^*}{\partial t^*} = \nabla^* \cdot (D_l^* \nabla^* c_l^* - \mathbf{u}^* c_l^*),\tag{1}$$

where t^*, D_l^* and $\mathbf{u}^*$ are time, the diffusivity of coffee within liquid and the velocity of the liquid respectively. The liquid flow should be solved for via the Navier-Stokes equations:

$$\frac{\partial \mathbf{u}^*}{\partial t^*} + (\mathbf{u}^* \cdot \nabla^*)\mathbf{u}^* = -\frac{1}{\rho^*}\nabla^* P^* + \frac{\mu^*}{\rho^*}\nabla^{*2}\mathbf{u}^*, \qquad \nabla^* \cdot \mathbf{u}^* = 0,\tag{2}$$

where μ^*, ρ^* and P^* are liquid viscosity, density and pressure respectively. Implicit in equations (2) are the assumptions that both the liquid density (so that the flow is incompressible) and viscosity are constant—in particular we take them to be independent of coffee concentration. We note that there is good evidence to suggest that the liquid density may vary appreciably during extraction. The act of extraction from espresso dissolves CO_2 which was trapped in the roasted bean. As a result the final product in the cup (i.e. a shot of espresso) has a density of approximately 0.7 relative to pure H_2O. This settles over time, as the CO_2 off gases. Nonethless, in the interests of simplicity, we elect to follow Moroney et al. [4] and adopt the constant density approximation.

Within each coffee grain the concentration of soluble coffee is governed by the following diffusion equation

$$\frac{\partial c_{si}^*}{\partial t^*} = \nabla \cdot (D_s^* \nabla^* c_{si}^*),\tag{3}$$

where D_s^* is the diffusivity of coffee within the solid coffee grains/cells. Motivated by the data shown in figure **??** we take the puck to be comprised of two different sizes of coffee grain

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with radii a_i for $i = 1, 2$ with $a_1 < a_2$. We therefore use the shorthand notation c_{si}^* to denote the concentration of coffee within the solid and will set the index $i = 1$ when discussing the smaller grains (c_{s1}^*) and $i = 2$ when discussing the larger grains (c_{s2}^*).

1.1 Boundary conditions

At the top of the bed we specify that the fluid pressure is equal to the pressure applied by the pump, that the tangential component of the liquid velocity is zero and that the normal liquid coffee flux should be zero, i.e.

$$P^*|_{z^*=0} = P_{tot}^*, \qquad \mathbf{u}^* \cdot \hat{\mathbf{t}}|_{z^*=0} = 0, \qquad (-D_l^* \nabla^* c_l^* + \mathbf{u}^* c_l^*) \cdot \hat{\mathbf{n}}\Big|_{z^*=0} = 0. \tag{4}$$

At the exit we apply conditions of zero (over) pressure, zero tangential velocity and an ad-hoc condition (that plays the role of a matching condition on the flux of coffee) to the one-phase region down stream of the basket. In other words, this final condition is based on the argument that, since extraction occurs only in the basket, in the stream of liquid that has left the basket the coffee concentration is independent of z and there is therefore no appreciable diffusive flux. In summary, we impose

$$P^*|_{z^*=L^*} = 0, \qquad \mathbf{u}^* \cdot \hat{\mathbf{t}}|_{z^*=L^*} = 0, \qquad (-D_l^* \nabla^* c_l^*) \cdot \hat{\mathbf{n}}\Big|_{z^*=L^*} = 0. \tag{5}$$

At the vertial edges of the cylindrical puck we apply no flux conditions on the liquid coffee concentration and no slip on the liquid velocity:

$$(-D_l^* \nabla^* c_l^* + \mathbf{u}^* c_l^*) \cdot \hat{\mathbf{n}}|_{R^*=R_0^*} = 0, \qquad \mathbf{u}^*|_{R^*=R_0^*} = \mathbf{0}. \tag{6}$$

On the boundaries between the grains and liquid — which we denote by Ω_i^* where $i = 1$ for the smaller grains and $i = 2$ for the larger grains — extraction of coffee takes place. We denote the flux of coffee concentration across these interfaces by G_i^*, so that appropriate boundary conditions are

$$(-D_s^* \nabla^* c_{si}^*) \cdot \hat{\mathbf{n}}|_{\Omega_i^*} = G_i^*, \qquad (-D_l^* \nabla c_l^* + \mathbf{u}^* c_l^*) \cdot \hat{\mathbf{n}}|_{\Omega_i^*} = G_i^*, \qquad \mathbf{u}^*|_{\Omega_i^*} = \mathbf{0}, \tag{7}$$

where the latter imposes no slip on the liquid velocity into the grains. We take the coffee extraction rate to be dependent on the concentrations local to the interface. Selecting a suitable reaction rate is non-trivial, however, it is clear that the rate should be zero when: (i) the liquid immediately outside the grain is saturated, i.e. at a concentration c_{sat}^*, or; (ii) when the liquid outside the grain is at the same concentration as the grain, or; (iii) when there is no coffee left within the grain. We therefore conjecture the following rate that satisfies these conditions, namely

$$G_i^* = k^* c_{si}^*|_{r^*=a_i^*} (c_{si}^*|_{r^*=a_i^*} - c_l^*)(c_{sat}^* - c_l^*) \tag{8}$$

where k^* is a rate constant.

1.2 Initial conditions

In real applications the packed bed of coffee grains is dry initially. The first step in extraction is to force liquid through the bed, wetting it, and also (perhaps) rearranging the grains within the bed, see [14]. Resolution of the initial stage poses a problem whose complexity is beyond the scope of the current work. We therefore circumvent this difficulty by assuming that at $t = 0$, the bed is filled with liquid water. We take

$$c_l^*|_{t^*=0} = 0, \qquad c_s^*|_{t^*=0} = c_{s0}^*. \tag{9}$$

Rearrangement of the geometry that may occur during the initial wetting stage will be accounted for later after the equations have been homogenised. One of the results of the procedure presented in §2 is replacing (2) with a statement of Darcy's law. In this equation the permeability of the bed appears, and by making it non-uniform in space we will be able to mimic non-uniform distributions of particles. Moreover, we will allow scope for the model to allow for the volume fractions and surface areas of the different phases to vary as a function of depth into the puck.

2 Homogenisation

In this section we carry out upscaling (or homogenisation) of the system of equations formulated in §1. Rather than resorting to a lengthy multiple scales analysis we use a combination of intuition and inspiration from the rigorous analysis presented in [22] to formulate the effective medium equations. Before proceeding we note the abuse of notation used in this section and henceforth; namely, that the dependent variables in §2 onwards are not the same as those appearing in §1 but are instead their upscaled counterparts. Despite this, in the interests of brevity of notation we opt not to make this distintion explicit.

Upscaling the Navier-Stokes equations (at suitable Reynolds numbers) on a porous media results in Darcy's law [11, 20], whilst upscaling (14) and accounting for the sources of c_l^* arising from the boundary conditions (7b) results in the following reaction-advection-diffusion equation [22]. We have

$$\mathbf{q}^* = -\frac{\kappa^*}{\mu^*}\nabla^* P^*, \qquad (1-\phi_s)\frac{\partial c_l^*}{\partial t^*} = \nabla^* \cdot \left(D_{eff}^*\nabla^* c_l^* - \mathbf{q}^* c_l^*\right) + b_{et,1}^* G_1^* + b_{et,2} G_2^*. \tag{10}$$

Here, κ^* is the permeability of the packed bed and $\mathbf{q}$ is the Darcy flux (i.e., the discharge per unit area with units of m/s) which is related to the average fluid velocity within the pore space, ν, via $q = (1-\phi_s)\nu$. One might conjecture that in espresso making applications pressures are sufficiently high, and the pores sufficiently small, that turbulent flow could be present. However, the experimental evidence strongly indicates that a model based on Darcy's law (rather than Ergun or Forchheimer [15, 18]) is suitable. In (10b), $b_{et,i}^*$ are the Brunauer-Emmett-Teller surface areas (defined to be the surface area, of grain species i, per unit volume of puck), and D_{eff}^* is the effective diffusivity which should be computed by via a suitable homogenisation procedure, see e.g. [16]. Alternatively one could approximate its

value using, e.g., Bruggeman's relation [12]. The quantity ϕ_s appearing in (10b) is the local volume fraction of coffee grains and is defined by

$$\phi_s = \phi_{s,1} + \phi_{s,2}, \quad \text{where} \quad \phi_{s,i} = \frac{b_{et,i}^*}{4\pi a_i^{*2}} \frac{4}{3} \pi a_i^{*3}. \tag{11}$$

The latter equation is a product of: (i) the surface area of particles per volume of bed divided by the surface area of a single particle— which is therefore the number of particles of a particular type per volume of bed, and; (ii) the volume of a single particle of a particular type. The product of these two factors is therefore the local volume fraction of the bed of particles of a particular size, and the sum over the terms gives the local solid volume fraction ϕ_s.

The form of the boundary and initial conditions to close (10b) remain unchanged, and are (4a), (5a), (6a) and (9a) but with $\mathbf{u}^*$ interchanged with $\mathbf{q}^*$. An important consequence of upscaling the Navier-Stokes equations to give Darcy's law is that the order of the system is reduced. We are therefore not at liberty impose all the boundary conditions laid out in §1. To close (10a) we retain (4b), (5b) and the component of (6b) normal to the boundary, i.e., $\mathbf{q}^* \cdot \hat{\mathbf{n}}|_{R^*=R_0^*} = 0$. The omission of the remaining conditions (namely (4c), (5c) and the tangential component of (6b)) is justified on the grounds that, had we carried out the homogenization explicitly, we would have imposed when solving on the microscopic length scale.

The governing equations for the coffee concentration in the solid phase remain unchanged by the homogenisation procedure; c_{si}^* are still to be determined by solving (3) with their associated boundary and initial conditions, (7a) and (9b). In the context of the multiple scales approach one can think of the retention of the full system for c_{si}^* as being necessitated by the need to evaluate the reaction rates, G_i^*, which can only be done by returning to the 'microscopic' scale. One must therefore solve two equations of the form (3) at each station in macroscopic coordinate system, one with $i = 1$ the other with $i = 2$, to predict the coffee conentration profiles within a 'representative' coffee grain of radius a_i^* (for $i = 1, 2$).

2.1 One-dimensional reduction

It follows from the form of the upscaled equations and boundary conditions that the solution should be one-dimensional, i.e., that it should dependent only on z^*, depth through the puck. In this case Darcy's equation reduces to

$$q^* = -\frac{\kappa^*}{\mu^*} \frac{\partial P^*}{\partial z^*}, \tag{12}$$

where the scalar q is the z-component of $\mathbf{q}^*$.

Since the primary focus of the model is to capture the extraction process after the initial wetting phase we assume that in the regime of interest the flow is steady. Despite this simplification we will provide scope for the model to capture consolidation of the bed that may occur in the wetting phase where the finer grains may be swept towards the bottom of

the puck by the intruding liquid — in the coffee making industry this process is known as fines migration. Importantly for our model such a phenomena would lead to spatial variations in the bed permeability. The solution to (12), with spatial dependence in κ^*, supplemented by the boundary conditions (4b) and (5b) is

$$q^* = \frac{\kappa^*_{eff} P^*_{tot}}{\mu^* L^*}, \qquad \kappa^*_{eff} = \frac{1}{L^*} \int_0^{L^*} \kappa^*(s^*) ds^*. \tag{13}$$

Inserting the result (13) into (10) and reducing to dependence only on z^* gives the following equation for c^*_l:

$$(1 - \phi_s) \frac{\partial c^*_l}{\partial t^*} = \frac{\partial}{\partial z^*} \left(D^*_{eff} \frac{\partial c^*_l}{\partial z^*} - \frac{\kappa^*_{eff} P^*_{tot}}{\mu^* L^*} c^*_l \right) + b^*_{et,1} G^*_1 + b^*_{et,2} G^*_2, \tag{14}$$

which is closed by the upscaled and reduced versions of (4a) and (5a), namely

$$-D^*_{eff} \frac{\partial c^*_l}{\partial z^*} + \frac{\kappa^*_{eff} P^*_{tot}}{\mu^* L^*} c^*_l \Big|_{z^*=0} = 0, \qquad -D^*_{eff} \frac{\partial c^*_l}{\partial z^*} \Big|_{z^*=L^*} = 0. \tag{15}$$

On assuming radial symmetry within each coffee grain the resulting problems to be solved for c^*_{s1} and c^*_{s2} are

$$\frac{\partial c^*_{si}}{\partial t^*} = \frac{1}{r^{*2}} \frac{\partial}{\partial r^*} \left(r^{*2} D^*_s \frac{\partial c^*_{si}}{\partial r^*} \right), \tag{16}$$

with boundary conditons (that arise from (7a)

$$-D^*_s \frac{\partial c^*_{si}}{\partial r^*} \Big|_{r^*=0} = 0, \qquad -D^*_s \frac{\partial c^*_{si}}{\partial r^*} \Big|_{r^*=a_i} = G^*_i. \tag{17}$$

The problem is closed by supplying the initial conditions (9).

2.2   Conservation of coffee in the upscaled problem

For the purposes of comparing model results to experimental data, which is typically presented as an extraction yield, it is necessary to consider how the coffee mass is conserved in the homogenised system. The total amount of coffee within the liquid phase at time t^* is given by

$$M^*_l = \pi R^{*2}_0 \int_0^{L^*} (1 - \phi_s) c^*_l dz^*. \tag{18}$$

On differentiating the equation above with respect to time, substituting (14) and evaluating the integral using the boundary conditons (15) we find that

$$\frac{dM^*_l}{dt^*} = -\pi R^{*2}_0 \frac{\kappa^*_{eff} P^*_{tot}}{\mu^* L^*} c^*_l \Big|_{z^*=L^*} + \pi R^{*2}_0 \int_0^{L^*} \left(b^*_{et,1} G^*_1 + b^*_{et,2} G^*_2 \right) dz^*. \tag{19}$$

5

The initial condition (9a) implies that

$$M_l^*|_{t^*=0} = 0. \tag{20}$$

Similarly, the total amount of coffee within the small ($i = 1$) or large ($i = 2$) grains at time t is

$$M_{si}^* = \pi R_0^{*2} \int_0^{L^*} \frac{b_{et,i}^*}{4\pi a_i^{*2}} \int_0^{a_i^*} 4\pi c_{si}^* r^{*2} dr^* dz^*. \tag{21}$$

On differentiating with respect to time, using equation (16) and boundary conditions (17) we find that

$$\frac{dM_{si}^*}{dt^*} = -\pi R_0^{*2} \int_0^{L^*} b_{et,i}^* G_i dz^* \tag{22}$$

The initial conditions (9b) requires that

$$M_{si}^*|_{t^*=0} = \pi R_0^{*2} c_{s0}^* \int_0^{L^*} \frac{b_{et,i}^*}{4\pi a_i^{*2}} \frac{4}{3}\pi a_i^{*3} dz^*. \tag{23}$$

On taking the sum of the equations (19) and (22), with both $i = 1, 2$, we find the following expression for the time rate of change of the total amount of coffee in the system

$$\frac{d}{dt^*}\left(M_l^* + M_{s1}^* + M_{s2}^*\right) = -\pi R_0^{*2} \frac{\kappa_{eff}^* P_{tot}^*}{\mu^* L^*} c_l^*\bigg|_{z^*=L^*}. \tag{24}$$

Initial data for the ODE above can be formulated by taking the sum of (20) and (23), with both $i = 1, 2$, and then using (11) to give

$$\left(M_l^* + M_{s1}^* + M_{s2}^*\right)\bigg|_{t^*=0} = \pi R_0^{*2} c_{s0}^* \int_0^{L^*} \phi_s dz^*. \tag{25}$$

Later, we will set out a numerical scheme to solve the model. The analytical expressions derived above for the rate of change of the total amount of coffee within each phase will serve as verification that the scheme is performing as expected.

Calculating the extraction yield For the purpose of comparing model results to data it is helpful to be able to compute the extraction yield which is the mass of solubles in the beverage divided by the dry weight of grounds that were initially put in the basket. Since the mass of solubles must be globally conserving during brewing we must have that $M_l^* + M_{s1}^* + M_{s2}^* + M_{cup}^*$ is constant, where M_{cup}^* is the mass of solubles in the cup. It follows from (24) that

$$\frac{dM_{cup}^*}{dt^*} = \pi R_0^{*2} \frac{\kappa_{eff}^* P_{tot}^*}{\mu^* L^*} c_l^*\bigg|_{z^*=L^*}. \tag{26}$$

6

This can be integrated, along with the initial condition that there is no beverage in the cup initially to give

$$M_{cup}^* = \pi R_0^{*2} \frac{\kappa_{eff}^* P_{tot}^*}{\mu^* L^*} \int_0^{t^*} c_l^* \Big|_{z^*=L^*} dt^*. \tag{27}$$

An expression for the extraction yield is arrived at by dividing this relationship through by the mass of dry grounds in the basket, $\phi_s \pi R_0^{*2} L^* \rho_{grounds}^*$, which leads to

$$EY = \frac{\kappa_{eff}^* P_{tot}^*}{\phi_s \rho_{grounds}^* \mu^* L^{*2}} \int_0^{t^*} c_l^* \Big|_{z^*=L^*} dt^*. \tag{28}$$

3   Nondimensionalisation

We now introduce suitable scalings for the variables in the problem. We scale by setting

$$z^* = L^* z, \quad t^* = \tau_{shot}^* t, \quad c_l^* = c_{sat}^* c_l, \quad c_{si}^* = c_{s0}^* c_{si}, \quad G_i^* = \frac{c_{sat}^*}{\tau_{shot}^* b_{et,0}^*} G_i, \quad r_i^* = a_i^* r_i. \tag{29}$$

Here, the timescale τ_{shot}^* is the time taken to pour a shot of espresso (typically around $20-30$s). Applying the scalings (29) introduces the following dimensionless parameters that characterise the system:

$$D_{eff} = \frac{D_{eff}^* \tau_{shot}^*}{L^{*2}}, \quad D_{si} = \frac{D_s^* \tau_{shot}^*}{a_i^{*2}}, \quad Q_i = \frac{1}{a_i^* b_{et,0}^*}, \quad \beta = \frac{c_{sat}^*}{c_{s0}^*}, \tag{30}$$

$$K = k^* c_{s0}^{*2} \tau_{shot}^* b_{et,0}^*, \quad b_{et,i} = \frac{b_{et,i}^*}{b_{et,0}^*}, \quad \nu = \frac{\kappa_{eff}^* P_{tot}^* \tau_{shot}^*}{\mu^* L^{*2}}, \quad \alpha = \frac{c_{s0}^*}{\rho_{grounds}^*}. \tag{31}$$

Of those parameters whose meaning is not self-evident from their definition: D_{eff} is the ratio of timescales for brewing and diffusive transport in the liquid; D_{si} are the ratios of timescales of brewing to diffusive transport in the two differently sized particles; ν is the ratio of the Darcy flux in the liquid to the characteristic velocity associated with brewing (L^*/τ_{shot}^*), and; K is the ratio of the typical flux of coffee in the solid to the flux through the solid/liquid interface and could therefore be termed an inverse mass transfer Biot number. We note that, in principle, we could select $b_{et,0}^*$ in such a way that one of the dimensionless parameters (either $b_{et,1}$ or $b_{et,2}$) is set to unity. However, we elect not to do this to retain transparency. For definiteness we elect to set $b_{et,0}^* = b_{et,1}^*/2 + b_{et,2}^*/2$.

Having applied (29) to the governing equations, boundary and initial conditions we arrive

at the following dimensionless system:

$$(1 - \phi_s)\frac{\partial c_l}{\partial t} = \frac{\partial}{\partial z}\left(D_{eff}\frac{\partial c_l}{\partial z} - \nu c_l\right) + b_{et,1}G_1 + b_{et,2}G_2, \tag{32}$$

$$-D_{eff}\frac{\partial c_l}{\partial z} + \nu c_l\Big|_{z=0} = 0, \qquad \frac{\partial c_l}{\partial z}\Big|_{z=1} = 0, \quad c_l|_{t=0} = 0, \tag{33}$$

$$\frac{\partial c_{si}}{\partial t} = \frac{1}{r_i^2}\frac{\partial}{\partial r_i}\left(r_i^2 D_{si}\frac{\partial c_{si}}{\partial r_i}\right), \tag{34}$$

$$-D_{si}\frac{\partial c_{si}}{\partial r_i}\Big|_{r_i=0} = 0, \qquad -D_{si}\frac{\partial c_{si}}{\partial r_i}\Big|_{r_i=1} = \beta Q_i G_i, \quad c_{si}|_{t=0} = 1, \tag{35}$$

where

$$G_i = Kc_{si}|_{r_i=1}\left(c_{si}|_{r_i=1} - \beta c_l\right)(1 - c_l). \tag{36}$$

Finally, it follows from (11), (24) and (25), that the statements of conservation of coffee become

$$\frac{dM_{tot}}{dt} = -\nu c_l\Big|_{z=1}, \qquad M_{tot}|_{t=0} = \frac{1}{\beta}\int_0^1 \phi_s dz, \qquad \phi_s = \frac{b_{et,1}}{3Q_1} + \frac{b_{et,2}}{3Q_2}. \tag{37}$$

where $M_{tot} = (M_l^* + M_{s1}^* + M_{s2}^*)/(\pi R_0^{*2} L^* c_{sat}^*)$. The dimensionless expression for the extraction yield (which is itself already a dimensionless quantity is)

$$EY = \frac{\nu\beta\alpha}{\phi_s}\int_0^t c_l|_{z=1}dt. \tag{38}$$

4 Numerical approach

Here, we describe an approach to numerically solve the dimensionless system of equations set out in §3, namely (32)–(36). The method centres around: (i) finite difference approximations of spatial derivatives in z; (ii) the use of a control volume method proposed in [24] for treatment of the spatial dependence in r; (iii) and, MATLAB's ODE suite for temporal integration.

Finite difference are the method of choice for the derivatives in z primarily for their ease of implementation. Zeng's control volume method [24] is particlularly apt to treat the transport of coffee in the solid phase for two reasons. Firstly, because it exhibits perfect conservation of 'mass'/coffee, which can be hard to ensure using standard finite differences owing to the singularity at the origin of the radial coordinate in the spherical diffusion equation. Secondly, in contrast to many other control volume methods, it provides direct access to the concentration on the surface of the particles thereby avoiding the need for extrapolation which would inevitably introduce additional errors. This surface concentration determines the reaction rate across the solid grain boundaries and so accurate evaluation of this quantity is crucial for reliable simulation. After applying these treatments for the

spatial dependencies, the system of PDEs (32)-(36) are reduced to system of coupled ODEs. We select the MATLAB routine `ode15s` to integrate this system forward in time because: (i) it is able to cope with a solving a system of differential-algebraic equations; (ii) it offers adaptive time-stepping, and; (iii) has relatively modest computational cost.

We introduce N equally spaced grid points, z_j for $j \in [1, N]$, thereby dividing the spatial z-domain into $N - 1$ equally spaced subdomains. The grid spacing in z is therefore given by $h_z = 1/(N-1)$. Henceforth we adopt the shorthand notation $c_l(z, t)|_{z=z_j} = c_{l,j}(t)$. At each station in z we must solve for the coffee concentration within a representative grain, *i.e.* , at each z_j we must solve two equations of the form (34); one with $i = 1$ for c_{s1} and another with $i = 2$ for c_{s2}. Each of the $2N$ copies of equation (34) are discretised by introducing M equally spaced grid points, r_k for $k \in [1, M]$, which subdivide each r-domain into $M - 1$ subdomains. The grid spacing in r is therefore given by $h_r = 1/(M-1)$. In total we have $N \times M$ different stations in r and at these locations we denote the value of the coffee conentration in small and large particles using the following shorthands $c_{s1}(z, r, t)|_{z=z_j, r=r_k} = c_{s1,j,k}(t)$ and $c_{s2}(z, r, t)|_{z=z_j, r=r_k} = c_{s2,j,k}(t)$, respectively. Thus, the index j indicates the representative particle's position in z whereas k labels the radial position within a particular resspentative particle. The $(2M + 1) \times N$ unknown functions of time into one large column vector $\mathbf{u}(t)$ as follows

$$\mathbf{u}(t) = [\mathbf{c}_l(t)^{\mathrm{T}} \ \mathbf{c}_{s1,1}(t)^{\mathrm{T}} \ \mathbf{c}_{s1,2}(t)^{\mathrm{T}} \ \cdots \ \mathbf{c}_{s1,N}(t)^{\mathrm{T}} \ \mathbf{c}_{s2,1}(t)^{\mathrm{T}} \ \mathbf{c}_{s2,2}(t)^{\mathrm{T}} \ \cdots \ \mathbf{c}_{s2,N}(t)^{\mathrm{T}}]^{\mathrm{T}}. \quad (39)$$

Here a prime denotes a vector transpose. We now rewrite the problem in the form

$$\mathbf{M}\frac{d\mathbf{u}}{dt} = \mathbf{f}(\mathbf{u}), \quad (40)$$

where $\mathbf{M}$ is the mass matrix and $\mathbf{f}(\mathbf{u})$ is a nonlinear function which arises from the application of finite difference approximations (to the equations in z) and the control volume method (for the equations in r). The system of ODEs (40) is written in the standard form accepted by MATLABs `ode15s`.

Below we present the first N entries of the nonlinear function $\mathbf{f}(\mathbf{u})$ arising from the discretisation of (32) and its boundary conditions (33a,b). The remaining $2MN$ equations arising from applying control volumes to (34) are detailed in [24] and so in the interests of brevity we do not repeat them here. We have

$$M_{1,1} = 0, \qquad f_1 = -\frac{D_{eff}}{h_z}\left(-\frac{3}{2}u_1 + 2u_2 - \frac{1}{2}u_3\right) + u_1, \quad (41)$$

$$M_{i,i} = 1 - \phi_s, \qquad f_i = \frac{D_{eff}}{h_z^2}(u_{i+1} - 2u_i + u_{i-1}) - \nu\frac{u_{i+1} - u_{i-1}}{2h_z} + b_{et,1}K, \quad (42)$$

$$M_{N,N} = 0, \qquad f_N = -\frac{D_{eff}}{h_z}\left(\frac{1}{2}u_{N-2} - 2u_{N-1} + \frac{3}{2}u_N\right). \quad (43)$$

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