MOVING BOUNDARY PROBLEMS IN SOLID/LIQUID SEPARATION

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1. INTRODUCTION

A problem of widespread industrial and theoretical importance is the separation of fine solids from liquids. The suspended solids are consolidated under the influence of a body force applied to the particles, for example, gravitational force in gravity thickening or an applied pressure in a pressure filter. In this paper, we outine the dynamics of such problems using the settling of a suspension in a closed bottom container under the force of gravity - that is batch settling.

2. EQUATIONS FOR BATCH SETTLING OF FLOCCULATED SUSPENSIONS

Electrolyte or polymer flocculants when added to suspensions cause the formation of connected aggregate structures (flocs) which fall faster than single solid particles because of their larger mass-to-surface-area ratio. While flocculation speeds up the settling process, the consolidated bed forms an open network of these flocs whose average volume fraction is lower than that acheived by a unflocculated sedimenting suspension. Above a critical volume fraction the network has some properties of solids. In particular the network can support compressive stresses up to a compressive yield stress; above this value the network will irreversibly deform. The compressive yield stress $P_y(\phi)$ is defined as the value of the network (particle) pressure at which the flocculated suspension at volume fraction ϕ will no longer resist compression elastically and will irreversibly consolidate. $P_y(\phi)$ can be obtained experimentally as discussed elsewhere [3,5].

The equations of motion, with a constitutive equation describing the yielding of the solid network are given and discussed in Buscall and White [3] and Landman, White and Buscall [11]. In this paper, we will consider only the case when the suspension is initially fully networked, thus avoiding the complications of differing floc sizes in a pre-networked system.

A force balance on the particulate network in a volume element of the suspension is

$$-\frac{\Delta\rho\, g\, \phi\, r(\phi)}{u_0}(\mathbf{u} - \mathbf{w}) - \nabla p - \Delta\rho\, g\, \phi\, \hat{\mathbf{z}} = 0 \qquad (1)$$

The first term (see glossary for a list of symbols used) is the hyrodynamic drag exerted by the suspending fluid on the sedimenting particles. The function $r(\phi)$ is the hindered settling factor and accounts for hydrodynamic interactions between the particles. Experimental measurements [2,10] and some theoretical work [1] has established the relationship

$$r(\phi) = (1 - \phi)^{-4.5} \qquad (2)$$

for unflocculated suspensions. We use this form in the present calculation for want of a more appropriate expression. The second term in equation (1) is the net force that the surrounding particles exert by direct interaction on the particles of the volume element. For flocculated suspensions, which form a network (when $\phi > \phi_g$) p is the elastic stress in the network. The third term is the net gravitational force exerted on the particles (weight minus upthrust from the suspending fluid). As is usual, the inertial terms and the shear forces in the bulk of the fluid and those exerted by the container walls on the neighbouring suspension are assumed small compared to the terms in equation (1), and so are neglected.

Conservation of particle and fluid masses requires the continuity equations

$$\frac{\partial\phi}{\partial t} + \nabla \cdot (\phi\mathbf{u}) = 0 \qquad (3)$$

$$\frac{\partial (1 - \phi)}{\partial t} + \nabla \cdot \{ (1 - \phi) \, w \} = 0 \qquad (4)$$

Buscall and White [3] put forward the following constitutive equation as modelling the response of flocculated suspensions:

$$\frac{D\phi}{Dt} = \begin{cases} 0, & p < P_y(\phi) & (5a) \\ \kappa(\phi) \, [p - P_y(\phi)] & p \geq P_y(\phi) & (5b) \end{cases}$$

where the function $\kappa(\phi)$ is the dynamic compressibility of the system. The compressive yield stress $P_y(\phi)$ is the value of the network pressure at which the network under compression will start to irreversibly consolidate. By expanding the material derivative in equations (5) and using the continuity equation (3), the constitutive equation may be rewritten as

$$\nabla \cdot u = \begin{cases} 0, & p < P_y(\phi) & (6a) \\ -\dfrac{\kappa(\phi)}{\phi} [p - P_y(\phi)] & p \geq P_y(\phi) & (6b) \end{cases}$$

Now suppose that the suspension is contained in a closed bottom container. Usually plug flow is assumed. In fact, the assumption that ϕ does not vary much over a horizontal cross-section of the container leads to similar equations in the horizontally averaged velocities and pressure [11]. In summary then, with

$$u = - u \, \hat{z} \qquad \text{and} \qquad w = w \, \hat{z} \qquad (7)$$

the continuity equations together with the closed bottom conditions give

$$- \phi \, u + (1 - \phi) \, w = 0 \qquad (8)$$

Hence the fluid velocity w may be eliminated from equation (1) to give the system

$$\frac{\partial \phi}{\partial t} = \frac{\partial (\phi u)}{\partial z} \qquad (9)$$

$$u = \frac{u_0 \, (1 - \phi)}{r(\phi)} \left[1 + \frac{1}{\Delta \rho \, g \, \phi} \frac{\partial p}{\partial z} \right] \qquad (10)$$

$$\frac{\partial u}{\partial z} = \begin{cases} 0, & p < P_y(\phi) & \text{(11a)} \\ \dfrac{\kappa(\phi)}{\phi} [p - P_y(\phi)] & p \geq P_y(\phi) & \text{(11b)} \end{cases}$$

where the yield stress $P_y(\phi)$ will be a given monotonic increasing function of ϕ.

At time $t = 0$, we assume here that the system is fully networked and that ϕ is a constant ϕ_0. Here $\phi_0 > \phi_g$, where ϕ_g corresponds to the lowest volume fraction for which the flocculated particles are networked. Since the container bottom is closed

$$u(0, t) = 0 \tag{12}$$

and

$$\int_0^{H(t)} \phi(z,t)\, dz = \phi_0 \, H_0 \tag{13}$$

where $H(t)$ is the height of the sedimenting column, with $H(0) = H_0$. The network pressure at the top of the bed is clearly

$$p(H(t), t) = 0 \tag{14}$$

Consolidation cannot occur until the network pressure p has increased above $P_y(\phi_0)$. Hence there will be a region at the top of the column, $z_c(t) \leq z \leq H(t)$, where $p < P_y(\phi_0)$ so that the equations give that the volume fraction remains at ϕ_0 and all the particles fall at the same velocity

$$u = -\frac{dH}{dt} \tag{15}$$

In this region equation (10) can be solved for the pressure:

$$p(z, t) = \Delta\rho \; g \; \phi_0 \left[\frac{dH}{dt} \frac{r(\phi_0)}{u_0 (1 - \phi_0)} + 1 \right] [H(t) - z] \tag{16}$$

The position z_c, which marks the boundary between the falling zone ($\phi = \phi_0$) and the consolidation zone ($d\phi/dz > 0$, $\phi_0 < \phi < \phi(0,t)$) is the point at which the network pressure becomes equal to the compressive yield stress:

$$p(z_c(t), t) = P_y(\phi_0) \tag{17}$$

Hence, equation (16) gives an equation combining the total solids height and the critical height

$$P_y(\phi_0) = \Delta\rho \ g \ \phi_0 \left[\frac{dH}{dt} \ \frac{r(\phi_0)}{u_0 \ (1 - \phi_0)} + 1 \right] \left[H(t) - z_c(t) \right] \tag{18}$$

Figure 1 shows a schematic illustration of the three zones in the consolidating column.
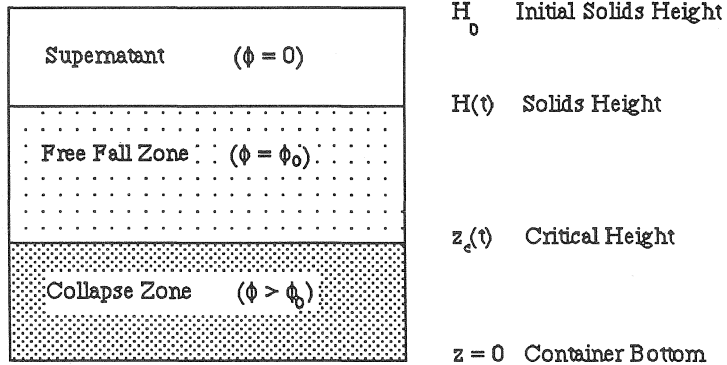
Figure 1: Schematic illustration of a consolidating sediment.

The equations to be solved in the consolidation zone $0 < z < z_c(t)$ are (9), (10) and (11b) with the conditions

$$\phi(z, 0) = \phi_0 \tag{19a}$$

$$u(0, t) = 0 \tag{19b}$$

$$\phi(z_c(t), t) = \phi_0 \tag{19c}$$

$$u(z_c(t), t) = -\frac{dH}{dT} \tag{19d}$$

$$p(z_c(t), t) = P_y(\phi_0) \tag{19e}$$

where we have assumed that the volume fraction, velocity and pressure are continuous at the interface between the falling and consolidation zones.

We consider now the large dynamic compressibility approximation to the consolidation equations. When $\kappa(\phi)$ is 'large', it follows immediately from equation (6b) that

$$p \cong P_y(\phi) \tag{20}$$

(almost) everywhere in the collapsing part of the sediment. Physically, when p exceeds $P_y(\phi)$, collapse is assumed so rapid that, locally, ϕ moves immediately to the value at which $P_y(\phi)$ exactly balances the applied network pressure. Network pressure can then never greatly exceed the yield stress in a rapidly collapsing structure. Therefore equation (11b) can be replaced with $p = P_y(\phi)$ and used directly in equation (10) to give a differential equation in ϕ. There will be a boundary layer in the neighbourhood of $z_c(t)$ which resolves the discontinuity in the z-derivative of ϕ [11].

Equation (20) is not new. Several authors [4,7,8] have made use of a constitutive equation connecting network stress to local volume fraction. Stable suspensions obey a constitutive equation $p = P_{os}(\phi)$ since the network pressure is just the osmotic pressure of the particles, which thermodynamically is a function of ϕ only. It should be understood, however, that the existence of a constitutive relationship for a flocculated suspension is predicted on the assumption of rapid collapse when the yield stress is exceeded.

3. DIMENSIONLESS SEDIMENTATION EQUATIONS

The equations may be made dimensionless by applying the following scalings:

$$Z = \frac{z}{H_0} \quad , \quad Z_c(T) = \frac{z_c(t)}{H_0} \quad , \quad L(T) = \frac{H(t)}{H_0} \tag{21a}$$

$$T = \frac{t\, u_0\, (1 - \phi_0)}{r(\phi_0)\, H_0} \tag{21b}$$

$$\Phi(Z,T) = \frac{\phi(z,t)}{\phi_0} \tag{21c}$$

$$U(Z,T) = \frac{u(z,t)\, r(\phi_0)}{u_0\, (1 - \phi_0)} \tag{21d}$$

$$f(\Phi) = \frac{P_y(\phi)}{P_y(\phi_0)} \tag{21e}$$

$$B(\Phi) = \frac{(1 - \phi_0 \Phi)\, r(\phi_0)}{(1 - \phi_0)\, r(\phi_0 \Phi)} \tag{21f}$$

$$\varepsilon = \frac{P_y(\phi_0)}{\Delta\rho\, g\, \phi_0\, H_0} \tag{21g}$$

For a consolidation zone to exist, $\varepsilon < 1$ [3].

For convenience the scaled sedimentation equations (in the large dynamic compressibility limit) are written in terms of Φ and the dimensionless solids flux $Q = \Phi U$. Then in $0 < Z < Z_c(T)$

$$\frac{\partial Q}{\partial Z} = \frac{\partial \Phi}{\partial T} \tag{22}$$

$$\frac{\partial \Phi}{\partial Z} = \frac{1}{\varepsilon\, f'(\Phi)\, B(\Phi)} \left[Q - \Phi B(\Phi) \right] \tag{23}$$

with boundary conditions

$$\Phi(Z, 0) = 1 \qquad\qquad (24a)$$

$$Q(0, T) = 0 \qquad\qquad (24b)$$

$$\Phi(Z_c(T), T) = 1 \qquad\qquad (24c)$$

$$Q(Z_c(T), T) = -\frac{dL}{dT} \qquad\qquad (24d)$$

subject to the condition

$$\left[1 + \frac{dL}{dT}\right]\left[L(T) - Z_c(T)\right] = \varepsilon \qquad\qquad (25)$$

An algorithm for solving the system (22)-(25) for the unknown functions $\Phi(Z,T)$, $Q(Z,T)$, $L(T)$ and $Z_c(T)$ is presented below.

4. TIME DISCRETISED EQUATIONS

We begin by approximating all time derivatives that appear in the consolidation equations by backward differences so that the state of the system at each time step can be determined from the state at the preceding time step. An additional advantage of discretising in time is that it converts the partial differential equations (22) and (23) to a pair of ordinary differential equations, which can be efficiently and accurately solved using Runge-Kutta techniques. This approach has been used before on moving boundary problems [12].

Let ΔT be the time step size. Approximating all time derivatives by first-order backward differences we have

$$\frac{\partial \Phi}{\partial T} \approx \frac{\Phi(Z, T) - \Phi(Z, T - \Delta T)}{\Delta T} \qquad\qquad (26)$$

$$\frac{dL}{dT} \approx \frac{L(T) - L(T - \Delta T)}{\Delta T} \qquad\qquad (27)$$

Denote by the superscript K (K = 0, 1, 2,....) the value of a function at time $T^K = K\Delta T$ so $\Phi^K(Z) = \Phi(Z, K\Delta T)$, and similarly for $Q^K(Z)$, L^K and Z_c^K. From the initial time state of the system, we have

$$\Phi^0(Z) = 1, \qquad L^0 = 1 \tag{28}$$

Discretising this way, the problem has been changed from one of finding the functions $\Phi(Z, T)$, $Q(Z, T)$, $L(T)$ and $Z_c(T)$ to one of finding the sequences $\Phi^K(Z)$, $Q^K(Z)$, L^K and Z_c^K. We will call the set $\{\Phi^K(Z), Q^K(Z), L^K, Z_c^K\}$ the Kth time state of the system. The equations to be solved in the region $0 < Z < Z_c^K$ are

$$\frac{dQ^K}{dZ} = \frac{\Phi^K - \Phi^{K-1}}{\Delta T} \tag{29}$$

$$\frac{d\Phi^K}{dZ} = \frac{1}{\varepsilon\, f'(\Phi^K)\, B(\Phi^K)} \left[Q^K - \Phi^K B(\Phi^K) \right] \tag{30}$$

subject to initial conditions (28) and

$$Q^K(0) = 0 \tag{31a}$$

$$\Phi^K(Z_c^K) = 1 \tag{31b}$$

$$Q^K(Z_c^K) = -\left[\frac{L^K - L^{K-1}}{\Delta T} \right] \tag{31c}$$

The equation connecting the interfaces of the two zones is

$$\left[1 - Q^K(Z_c^K) \right]\left[L^K - Z_c^K \right] = \varepsilon \tag{32}$$

after using equation (24d) in (25).

In the next section we describe a method whereby the Kth time state of the system may be determined given $\Phi^{K-1}(Z)$ and L^{K-1}, that is data from the $(K-1)^{th}$ time state. Then since $\Phi^0(Z)$ and L^0 are known, all time states for $K > 0$ may be determined inductively.

5. A RUNGE-KUTTA SHOOTING METHOD

Equations (29)-(30) are two coupled first-order ordinary differential equations which may be solved by Runge-Kutta

integration, but the particular method of solution depends on the nature of the boundary conditions. The no-flux condition (31a) is a simple boundary condition. The conditions (31b,c) at the other boundary, together with (32), specify Q^K and Φ^K in terms of Z_c^K and L^K. But Z_c^K and L^K are unknown. We therefore regard these three equations as 'one' boundary condition at Z_c^K. It is this fact which introduces complexity into the numerical scheme.

In order to solve any two-point boundary value problem where the range of integration is known, a Runge-Kutta shooting method is commonly used. Here the upper limit of the range of integration is unknown so that we must adapt such a shooting algorithm. Below is a description of the procedure which is implemented for each fixed K.

(1) We define a mesh on the Z interval [0,1] by dividing that interval into N subintervals of width ΔZ.

(2) We guess the value of $\Phi^K(0)$. With the given boundary condition $Q^K(0) = 0$, we now have an initial value problem, which can be solved numerically using the 4th order Runge-Kutta method.

(3) We continue integrating in Z until we reach a Z-value for which $\Phi^K(Z) = 1$. This gives an estimate of Z_c^K and call this value Z^*.

(4) In the course of the integration, $Q^K(Z^*)$ will be determined. This value is used in (31c) to give a value for L^K. Then substitution of both $Q^K(Z^*)$ and L^K into (32) yields a second estimate for Z_c^K, which we call Z^{**}.

(5) We now have two numbers, Z^* and Z^{**} as estimates of Z_c^K. If the guess $\Phi^K(0)$ is a good one, then Z^* and Z^{**} should agree, within an assigned tolerance, e.g.

$$\left| \frac{Z^{**}}{Z^*} - 1 \right| < \text{TOLERANCE} \qquad (33)$$

If this is the case, set $Z_c{}^K = Z^*$ and the values of L^K, $Q^K(Z)$ and $\Phi^K(Z)$ just determined give the required K^{th} time state of the system. On the other hand, if the convergence criterion is not met, then we must guess another value of $\Phi^K(0)$ and repeat the steps 2 − 5. Continue in this way with guessed values until the convergence criterion is satisfied. The method for choosing each $\Phi^K(0)$ is described in detail elsewhere [9].

6. NUMERICAL RESULTS

To exhibit the utility of this algorithim, we have performed numerical calculations on a model sedimenting network using two parameter (n,k) power law curves of the type

$$P_y(\phi) = k\left\{\left[\frac{\phi}{\phi_g}\right]^n - 1\right\} \tag{34}$$

with n between 4 and 10. Yield stresses of this form have been fitted by our experimental collaborators to systems such as polystyrene latex [13] and red mud suspensions [6]. Expressions of this form obey $P_y(\phi_g) = 0$, consistent with the definition of ϕ_g. Since we are only working with fully networked suspensions $\phi \geq \phi_0 \geq \phi_g$.

The functions $B(\Phi)$ and $f(\Phi)$ may be written explicitly in terms of these dimensionless variables using the forms for $r(\phi)$ (in equation (2)) and $P_y(\phi)$ above. Hence

$$B(\Phi) = \left[\frac{1 - \phi_0\Phi}{1 - \phi_0}\right]^{5.5} \tag{35}$$

and

$$f(\Phi) = \frac{C^n \Phi^n - 1}{C^n - 1}, \qquad C = \frac{\phi_0}{\phi_g} \tag{36}$$

where now C > 1.

In Figure 2 we plot the computed scaled volume fraction as a function of Z in the consolidating zone at various times. This allows the evolution of the consolidating bed to be observed. As well, Figure 3 shows the scaled bed height L(T) and the scaled critical height marking the consolidating zone $Z_c(T)$ as a function of time.

Note that in the volume fraction graph the horizontal axis is the line $\Phi = 1$, so that the point where the curves meet this line is the point $Z_c(T)$. Thereafter $\Phi = 1$ for $Z_c(T) \leq Z \leq L(T)$, where L(T) can be determined from the Fig 2b.

(i) The volume fraction profiles are concave upwards for early times, while for later times they are concave downwards, that is the second Z-derivative of Φ decreases with time and changes sign. This behaviour is anticipated from the analytic forms of the solution at small times and at equilibrium. These profiles are for fully networked suspensions, so that the differing floc sizes and shapes do not affect the sediment behaviour.

(ii) The $\sqrt{T}$ behaviour of $Z_c(T)$ for early times as derived elsewhere [9] is clearly illustrated. Also the approach of $\Phi(Z,T)$, L(T) and $Z_c(T)$ to their steady state equilibrium values can be clearly seen. The analytic forms of the steady state solution is also given in [9].

The effect of varying n, C and ε is gven in [9].Essentially, if one of n, C, or ε is varied, the yield stress of the network $P_y(\phi)$ is changed for $\phi > \phi_0$, the region of interest. Smaller values of $P_y(\phi)$ at a given concentration mean that the network is easier to compress, so we expect greater concentrations in a more compact consolidation zone.
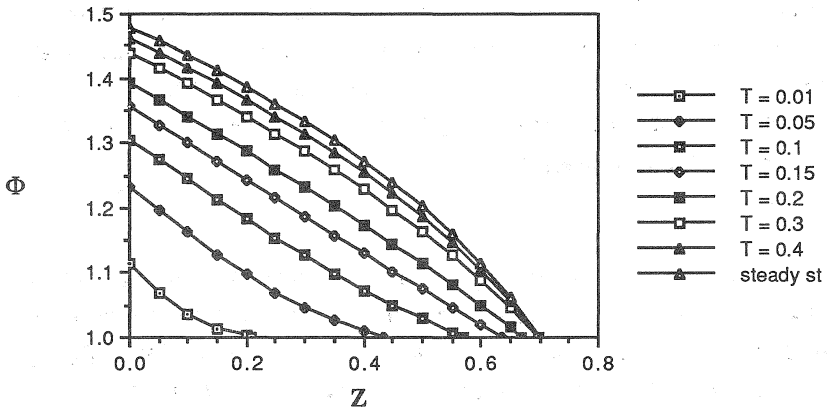
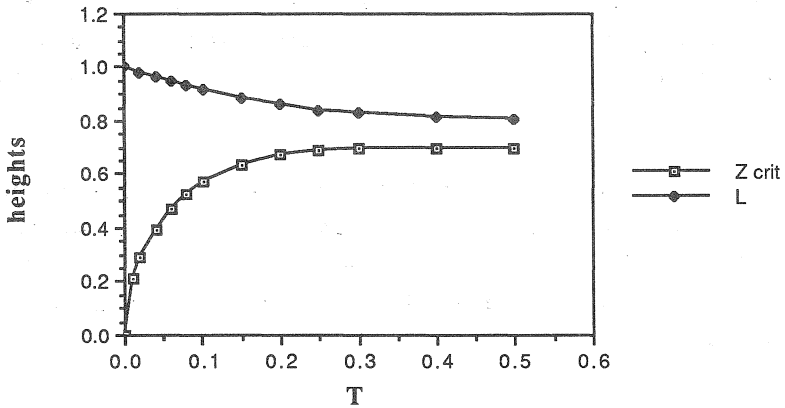**Figure 2:** Volume fraction profiles for n = 5, C = 1.25, $\varepsilon = 0.1$

Figure 3: Critical height $Z_c(T)$ and bed height $L(T)$ for n = 5, C = 1.25, $\varepsilon = 0.1$.

Corresponding asymptotes are $Z_{cs} = 0.7011$ and $L_s = 0.8011$

GLOSSARY TO SYMBOLS USED

LOWER CASE ROMAN

$f(\Phi)$	scaled yield stress function
g	gravitational constant
k	proportionality constant in yield stress function
n	index in yield stress function
p	network pressure
$r(\phi)$	hydrodynamic interaction factor
t	time
u	magnitude of solids velocity vector
u_0	Stokes settling velocity of an isolated particle
$\mathbf{u}$	solids velocity vector
w	magnitude of fluid velocity vector
$\mathbf{w}$	fluid velocity vector
z	vertical spatial coordinate
$z_c(t)$	critical height, boundary of the consolidation zone

UPPER CASE ROMAN

$B(\Phi)$	scaled hydrodynamic drag function
C	constant in $f(\Phi)$
H_0	initial solids height
$H(t)$	solids height
K	superscript labelling time steps
$L(T)$	scaled solids height
L^K	time discretised scaled solids height at the Kth time step
L_s	steady state scaled solids height
$P_y(\phi)$	yield stress of a flocculated suspension
Q	scaled solids flux
Q^K	time discretised scaled solids flux at the Kth time step
T	scaled time
T^K	time at the Kth time step
$U(Z,T)$	scaled downward solids speed
Z	scaled vertical spatial coordinate

z^* for each time step K, this is the estimate of Z_c^K obtained by the shooting method (31b)

z^{**} for each time step K, this is the estimate of Z_c^K obtained form equations (32)

$Z_c(T)$ scaled critical height

Z_c^K time discretised scaled critical height at the Kth time step

Z_{cs} steady state scaled critical height

LOWER CASE GREEK

ε dimensionless number characterising a flocculated suspension

ϕ volume fraction of suspension occupied by solids

ϕ_g gel point of a flocculated suspension

ϕ_0 initial volume fraction

$\kappa(\phi)$ dynamic compressibility of the flocculated network

UPPER CASE GREEK

$\Delta\rho$ difference between solid and fluid densities

ΔT time step size

ΔZ grid spacing on coarse mesh

$\Phi(Z,T)$ scaled solids volume fraction

$\Phi^K(Z)$ time discretised scaled solids volume fraction

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