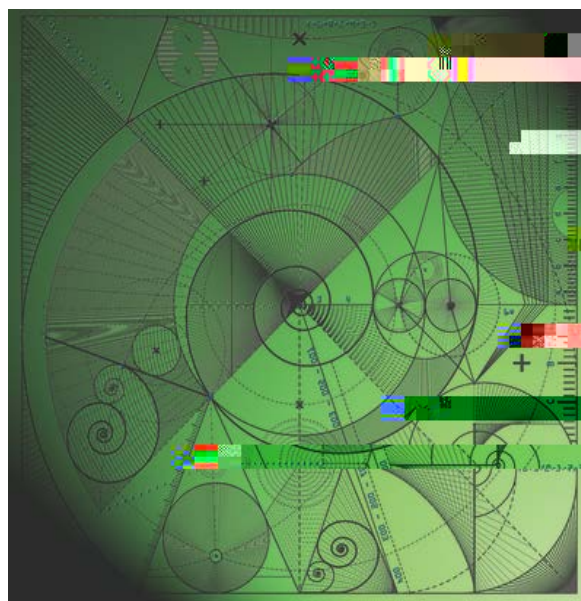


Capillary transport in particulate porous materials at low levels of saturation: the mathematical model and a comparison with experimental observations

by

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Capillary transport in particulate porous materials at low levels of saturation: the mathematical model and a comparison with experimental observations.

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We have established previously, in a pilot study, that the spreading of liquids in granular porous materials at low levels of saturation, typically less than 10% of the available void space, has very distinctive features in comparison to that at higher saturation levels. In particular, it has been shown, on theoretical grounds, that the spreading is controlled by a special type of diffusion process, that its physics can be captured by an equation of the super-fast diffusion class, and that these findings were supported by first-of-a-kind experiments. In this paper, we take these findings to the next level including deeper examination and exposition of the theory, an expanded set of experiments to address scaling properties, and systematic evaluations of the predictive performance against these experimental data, keeping in mind also potential practical applications.

I. INTRODUCTION

Even a small amount of a liquid added to a dry granular material may dramatically change its structural properties due to the appearance of a strong capillary cohesion force between the particles [1-4]. The strong capillary force, of the order of $F_c = 2R\sigma\cos\theta_c$, is due to the liquid bridges (pendular rings) formed at the point of particle contact [5, 6]. Here, R is the average particle radius, σ is the surface tension coefficient and θ_c is the static contact angle of the liquid formed at the three-phase contact line on the flat surface of the solid. A simple estimate for water at room temperature ($\sigma = 72 \text{ mN/m}$) and sand particles ($\theta_c = 30^\circ$) of $400 \text{ }\mu\text{m}$ in diameter results in $F_c = 8 \cdot 10^{-5} \text{ N}$, which is much larger than the gravity force acting on each particle $\approx 8 \cdot 10^{-8} \text{ N}$. It is interesting to note, that the cohesive force is practically independent of the liquid content, that is the value of saturation, as can be interpreted as the characteristic average thickness of the surface roughness. For example, a threshold value $s_0 = 0.2\%$ has been observed in experiments using spherical particles, average radius $R = 187.5 \text{ }\mu\text{m}$, with the maximum surface roughness amplitude of approximately 500 nm as determined by scanning force microscopy [1]. At the same time, in our experiments with Ottawa sands, average grain radius $R = 250 \text{ }\mu\text{m}$ with the surface roughness amplitude distributed between 250 nm and $3 \text{ }\mu\text{m}$ [9], a minimal value of $s_0 = 0.6\%$ was observed, implying an effective r_R value of $1.5 \text{ }\mu\text{m}$. One can see that the lower is the surface roughness on average, the lower is the critical value s_0 .

If we now consider spherical (or nearly spherical) grains and take into account that only some part of the volume $\frac{4}{3}R^3$ is available for the liquid during the spreading, then the value of saturation due to the liquid distributed

on the rough surface of the grains is

$$s_0 = 3 \frac{1}{R} \frac{R}{R}; \quad (1)$$

where parameter

Set	Liquid
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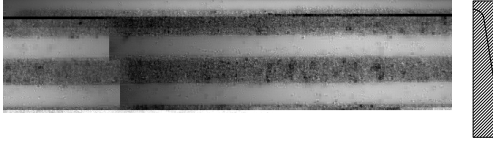


FIG. 6. Channels in Te on (diameter of the hemicylinder $d_c = 6.15$ mm) filled in by the standard Ottawa sand ($R = 0.25$ mm) before depositing $V_D = 3 \text{ mm}^3$ liquid drops.

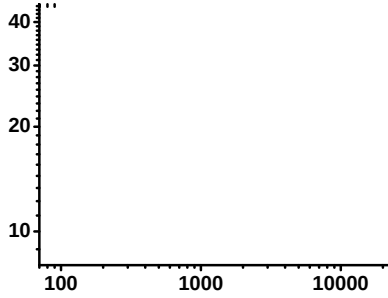


FIG. 7. Spreading of TCP, TEHP and TBP liquid drops ($V_D = 3 \text{ mm}^3$) in $R = 0.25$ mm sand in the channels, as in Fig. 6. Normalised wet volume $V = V_D$ (inverse average saturation s^{-1}) as a function of time. The experimental data are shown by symbols and the solid lines (brown) are the fits $V = V_D = A + Bt^{0.5}$.

Using (3) and (4), the average capillary bridge pressure $P = \langle p \rangle^I$ can be presented as

$$P = p_0 \frac{C_1 A_s^{1/2}}{(s - s_0)^{1/2}}; \quad (5)$$

where $\langle \dots \rangle^I = \frac{1}{V_l} \int_V \dots d^3x$ is intrinsic liquid averaging, V_l is liquid volume within the sample volume V . We have assumed previously in developing our preliminary theoretical model that parameter s_0 is constant, that is independent of the capillary pressure. This is a good approximation in a range of capillary pressures, but could be possibly violated at small values of $s_f - s_0$. Indeed, consider a model groove geometry shown in Fig. 8. Surface flows in that kind of geometry have been studied experimentally and theoretically in [10][12]. The liquid in this case is contained both inside the large scale grooves (large scale surface roughness), in capillary menisci, and on the surface with much smaller scale roughness. At very large capillary pressure, the meniscus curvature could be much

mensions [19, 20], obeys a Darcy-like law

$$q = -\frac{\mu}{\eta} r ; \quad (7)$$

where μ is liquid viscosity, η is local pressure in the liquid averaged within the surface roughness and $\eta_m = \eta_0 \frac{2}{R}$ is the effective coefficient of permeability of the surface roughness, which is proportional to the square of the length scale parameter R . To understand the order of magnitude of $\eta_m = \eta_0 \frac{2}{R}$, one can again consider the surface groove of a simplified geometry, as is shown in Fig. 8. We note, that the fluid flow mostly occurs within large scale surface grooves. Then, assuming a fully developed rectilinear Hagen-Poiseuille flow in the open channel at $\theta_0 = \pi/2$ and $\theta_c = 0$, Fig. 8, and the results of analysis of liquid flows in corners in [21], $\eta_0 = \frac{\eta_0}{1} \frac{1}{4}$, where non-dimensional parameter η_1 was found to be $\eta_1 \approx 100$ [21] and parameter $\eta_0 < 1$ is the ratio of the total cross sectional area of the grooves to the total cross sectional area of the surface layer of width R . Due to the capillary pressure variations in the grooves and, as a consequence, variations of the cross-section area of the groove volume occupied by the liquid, parameter η_0 would vary in the idealized case between $\frac{\eta_0}{1} \frac{1}{4}$ and $\eta_0 \frac{\eta_0}{2}$, where parameter η_2 in the case of a fully saturated groove was found to be $\eta_2 \approx 50$ [21]. This implies that $\eta_0 = \eta_0(s)$. When s changes from s_f to s_c , assuming again a linear relationship

$$\eta_0(s) = \frac{\eta_0^2}{s_c} \frac{1}{s_f} (s - s_f) + \frac{1}{\eta_0};$$

$$\frac{1}{\eta_0} = \frac{\eta_0}{1} \frac{1}{4} ; \quad \frac{2}{\eta_0} = \frac{\eta_0}{2}.$$

The minimum value of the channel permeability is defined by the maximum capillary pressure in the system. We note, while in unbounded V-shaped grooves, especially at small opening angles θ_0 , the free surface is also unbounded, so that the capillary spreading in the absence of external forces, like the gravity force, is unbounded, in our case, a quasi-steady state is observed corresponding to the maximum capillary pressure [22]. If the contact angle θ_c is not equal to zero, then the amount of the liquid contained in the groove at a fixed value of pressure, that is at a fixed value of η_R is reduced. Then

$$\frac{1}{\eta_0} = \frac{\eta_0}{1} \cos \theta_c (\cos \theta_c - \sin \theta_c) \approx 5.39 \cdot 0.14$$

To obtain analytical results, we restrict ourselves to the case of a spherical particle of radius R . In this case, domain boundaries ∂_1 and ∂_2 will be circular cross

and

$$v_{j@} = \frac{1}{s_f} \frac{u_0^{\frac{3}{2}}}{\ln u_0} \frac{\partial u}{\partial x_{@}} ; \quad (24)$$

where $u = s - s_f$ and u_0

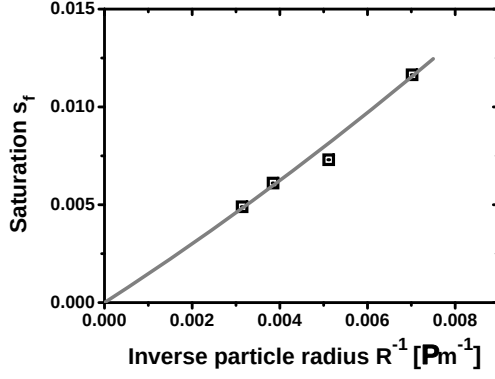


FIG. 10. Saturation s_f as a function of R^{-1} shown by symbols. The solid line is the $s_f = A_f R^{-1} + B_f R^{-2}$ at $A_f = 1.5 \text{ m}$ and $B_f = 29 \text{ m}^2$.

can present (22) in non-dimensional form by normalizing distances $x = x/L_0$ and time $t = t/t_0$. As the characteristic length scale, we use the wet spot radius L_0 at some moment of time, which will be initial time for simulations $t = 0$, and $t_0 = L_0^2/D_0^e$. Then, omitting tilde in the notations, equation (22) can be presented as

$$\frac{\partial s}{\partial t} = r \frac{c_0(s) r s}{j \ln(s - s_0^e) j (s - s_0^e)^{3=2}} ; \quad (26)$$

with two boundary conditions

$$s|_{@} = s_f \quad (27)$$

and

$$v_n j|_{@} = \frac{c_0(s) (n - r) s}{s_f j \ln(s_f - s_0^e) j (s_f - s_0^e)^{3=2}}. \quad (28)$$

Here

$$D_0^e = \frac{3}{R^2} - \frac{1}{0} \frac{P_c}{c} \quad (29)$$

and

$$c_0(s) = \frac{\frac{2}{0} - \frac{1}{0}}{s_c - s_0^e} \frac{1}{s_0^e} (s - s_0^e) + 1$$

in

$$s_0^e \leq s \leq s_c$$

otherwise

$$c_0(s) = \frac{2}{0} - \frac{1}{0}.$$

So, the problem has three essential non-dimensional parameters s_f , $s_f - s_0^e$ and $V_D = L_0^3$. The last parameter only contributes through the initial profile of saturation $s(x; 0)$ at $t = 0$. We have already seen that variations of initial drop volume V_D at $s_f = \text{const}$ and $s_f - s_0^e = \text{const}$ result

in self-similar behaviour, such that evolution curves of the moving front collapse on a single master curve after re-normalizing time t by a factor of $V_D^{2=3}$. This implies that one can further assume that L_0^3 / V_D , so that parameter L_0 can be solely defined by the initial drop volume V_D . This leaves us with just two non-dimensional

$$\frac{\partial s}{\partial t} = r \frac{c_0(s) g(s) r s}{j \ln(s - s_0^e) j (s - s_0^e)^{3/2}} ; \quad (30)$$

where augmenting permeability function $g(s)$, Fig. 11,

$$g(s) = 1 + f_0 10^{-g s} \quad (31)$$

with

$$g = 16.5; \quad g = 1.65$$

and

$$f_0 = \frac{R}{R_m}^2 - \frac{w}{w} ; \quad (32)$$

The values of the coefficients in (31) have been chosen such that, according to [31], in the medium fine sands ($R_m = 260 \text{ m}$) and water (surface tension w and viscosity w)

$$g(s) \big|_{s=0.1} = 2; \quad g(s) \big|_{s=0.3} = 2000$$

and $f_0 = 1$. As one can see, Fig. 11, the augmenting function $g(s)$ due to the strong decline with the saturation has a very short crossover region quickly reaching a constant value $g(s) = 1$ at $s = 0.1$, where the pendular regime begins. We note that we still use pressure-saturation relationship (6), which provides a reasonable approximation considering strong variations of permeability. Alternatively, the model can be easily generalized by using a Leverett J-function [32].

D. Numerical simulations and experimental results in three-dimensional spherically symmetric cases

To compare numerical solutions of the superfast diffusion model (30) with experimental observations, we first consider simulations in a three-dimensional spherically symmetric case, where saturations $s(r; t)$ is a function of time and the radius r in a spherical coordinate system with its origin at the centre of the hemisphere representing the wet volume, Fig. 4. We have started our simulations in this case with

$$s(r; t) \big|_{t=0} = s_f + s_a \cos^a(r/2); \quad 0 \leq r \leq 1 \quad (33)$$

at different values of parameters $0.2 \leq s_a \leq 1$, s_f and $0.2 \leq a \leq 0.4$. The value of L_0 then is defined by conservation of the liquid, neglecting the evaporation effects,

$$2 \int_0^1 s(r; 0) r^2 dr = V_D L_0^3;$$

We note, that due to the use of a spherical coordinate system, we also require that at $r = 0$ the first derivative $\partial s / \partial r = 0$ to avoid singular spurious solutions.

The choice of parameters s_a in the initial distribution and even its functional form is not obvious. We observed in the experiments that just in about ten minutes of spreading, the wetting spot volume shape becomes

FIG. 12. Simulation of spreading in a three-dimensional spherically symmetric case using augmented superfast diffusion model (30) with initial distribution (33) at $s_a = 0.3$, $s_a = 0.4$, $g = 16.5$; $g = 1.65$; $f_0 = 1$ and $s_f = 0.0052$, but at different values of parameter $s_f - s_0^e$. Normalised wet volume $V = V_D$ (inverse average saturation s^{-1} , solid lines) as a function of the reduced time $t = t_0$, $t_0 = L_0^2 / D_0^0$. From left to right: (I) $s_f - s_0^e = 0.0001$, (II) $s_f - s_0^e = 0.0002$, (III) $s_f - s_0^e = 0.0004$, (IV) $s_f - s_0^e = 0.0008$. Insert shows the power law $V = V_D = A + B(t = t_0)^{0.75}$ (solid line, brown) in comparison with the numerical data (symbols, black) at $s_f - s_0^e = 0.0008$.

spherically symmetric, when the average saturation level $s = 0.5$, Fig. 5. But what is the liquid distribution at this stage?

If we fix parameters of the initial distribution (s_a and a) and parameter s_f , then evolution of the moving front at different values of $s_f - s_0^e$ represents a family of curves shown in Fig. 12. One may notice that, first of all, the smaller is the parameters $s_f - s_0^e$ (that is the higher is the reduced capillary pressure at the moving front) the faster the spreading occurs. Secondly, the power law found in the experiments $V = A + B(t = t_0)^{0.75}$ is very well observed in the simulations, see insert in Fig. 12.

As one can see from the distribution of the liquid at $t > 0$, Fig. 13 (a)-(b), the saturation profile quickly relaxes to a universal distribution at fixed values of s_f , $s_f - s_0^e$ and V_D . The distribution $s(r; t)$ at $t = t_2 = 6 \cdot 10^{-5}$, when the average value of saturation is already $s = 0$:

FIG. 13. Simulation of spreading in a three-dimensional

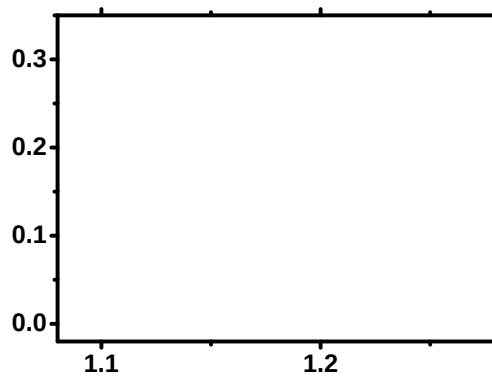
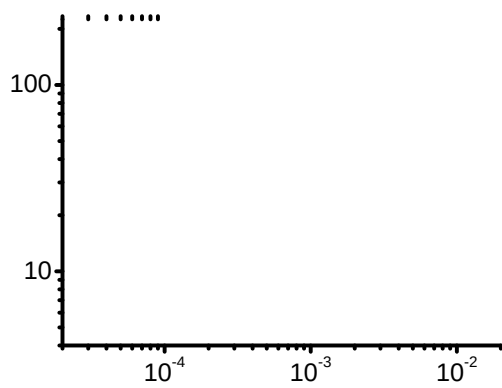


FIG. 14. Simulation of spreading in a three-dimensional spherically symmetric case using augmented superfast diffusion model (30) with initial distributions given by (33) at $s_a = 0.2$ and $s_a = 0.5$. Saturation $s(r; t)$ as a function of the reduced spot radius $r=L_0$ at fixed values of $\eta_g = 16.5$; $\eta_g = 1.65$; $f_0 = 1$, $s_f = 0.0052$ and $s_f = s_0^e = 0.0002$. A comparison between the asymptotic solution (34) (solid line, brown) and the numerical solution at $t = t_1 = 3 \cdot 10^{-6}$ shown by symbols, $W_0 = 287$. The insert shows a similar comparison, but at $t=t_0 = t_2 = 6 \cdot 10^{-5}$, $W_0 = 62$.

general case

$$X_n(t) / t^{1-(n+1)} ;$$



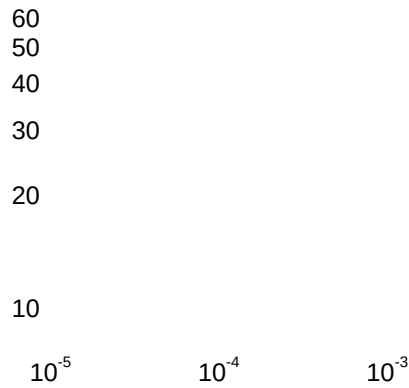


FIG. 17. Spreading TCP, TEHP and TBP liquid drops ($V_D = 3 \text{ mm}^3$) in sands with $R = 0.25 \text{ mm}$ in one-dimensional geometry. Comparison between experimental data and simulations using superfast diffusion model (30) with initial distribution of saturation given by (35). Normalised wet volume $V = V_D$ (inverse average saturation s^{-1}) as a function of the reduced time $t = t_0$, $t_0 = L_0^2/D_f$. Experimental data are shown by symbols and simulation is presented by the solid line. Parameters of the simulations and the fitting are summarized in Table I. The dashed line (brown) is the $V = V_D = A + B(t=t_0)^{0.5}$ at $A = 8.5$ and $B = 440$.

expect that the distributions could be different due to the hysteresis effect commonly observed in porous media spreading processes [32, 34, 35]. For example, if some areas on the grain surfaces were inaccessible to the liquid flow at low saturation levels [11], then during shaking and mixing those areas might be wet. The assumption is in agreement with the analysis presented in [11] and our observations that the equilibrium value of $R = 0.2$ after natural spreading is small. That is, during the natural spreading, large surface areas of the grains were left dry. This implies that the liquid content in equilibrium would depend on the way this equilibrium was achieved, and this seemed to be observed in our experiments, Figs.

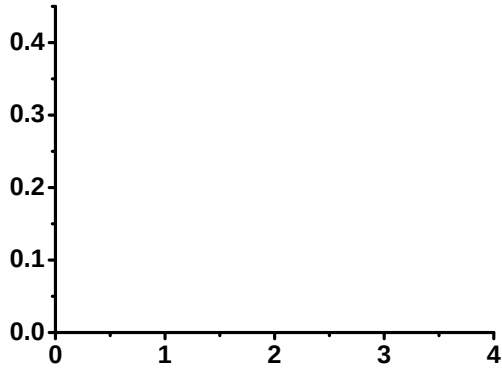


FIG. 20. Simulation of spreading of TEHP liquid drops ($V_D = 6 \text{ mm}^3$) in pre-wetted sands with the background saturations level $s_r = 1\%$ using the augmented model (30) with initial conditions (36) at $s_a = 0.4$, $r_a = 4$ and $\alpha_a = 0.3$ with $s_0^e = 0.0068$.

Hence, one can easily follow the evolution of a benchmark point $x_m(t)$, as is shown in Fig. 20. The result at $s_r = 1\%$, shown in Fig. 19 in terms of the evolution of the volume contained within $0 \leq r \leq x_m$, indicates that while there is some initial plateau in the distribution of the saturation, as is observed in the experiments presented in the same figure, in general the evolution is much slower. One can conclude then that, while the initial plateau observed during the volume evolution at high average saturation values $\approx 20\%$ at both $s_r = 2\%$ and $s_r = 1\%$ indicates that the mechanism of spreading is sensitive to the background levels, see Fig. 19, to the large extent the spreading dynamics is still defined by the front capillary pressure generated on the scale of surface roughness. One can also conclude that the liquid morphology of that background liquid distribution seemed to be different from the liquid morphology observed at these saturation levels during the natural spreading.

In the second case, $s_r < s_0^e$, one needs to modify the original model to include the presence of some background saturation level. Using conservation of the liquid in the domain with a front $@(t)$ moving into the area with background saturation s_r and the transport Reynolds theorem

$$\frac{d}{dt} \int_{(t)} s d^3x = \int_{(t)} \frac{\partial s}{\partial t} + r \cdot (sv) d^3x =$$

$$= \int_{@(t)} (v \cdot n) s_r dS;$$

where n is the normal vector to $@$.

Transforming the surface integral into the volume in-

tegral

$$\int_{(t)} \frac{\partial s}{\partial t} + r \cdot ((s - s_r)v) d^3x = 0:$$

This implies that an equivalent moving boundary-value non-linear diffusion problem of transport in pre-wetted sands can be formulated in terms of a function $s = s_r$

$$\frac{\partial s}{\partial t} = r \frac{c_0(s) g(s) r}{j \ln(s - s_0) j (s - s_0)^{3/2}}; \quad (37)$$

$$s_0 = s_0^e - s_r$$

with the boundary conditions

$$j_{@} = s_f - s_r$$

and

$$v_n j_{@} = \frac{c_0(s) g(s) r}{(s_f - s_r) j \ln(s_f - s_0^e) j (s_f - s_0^e)^{3/2}}; \quad (38)$$

One can see that in general due to a smaller factor at the moving front $s_f - s_r$ (instead of just s_f), the front motion is expected to proceed with much higher velocity.

This is understandable, since one requires (is)-336ts understandable

CONCLUSIONS

In our previous study we established that:

The process of spreading can be described by a special type of non-linear diffusion process, where the driving force is the capillary pressure at the moving front generated by the particle surface roughness and the coefficient of diffusion has a characteristic singular form $D(s) \propto (s - s_0^e)^{-3/2}$. The resulting mathematical model belongs to a class known as super-fast diffusion equation, and the so-suggested scaling with viscosity and surface tension is as expected for capillary flows, $D \propto \eta \gamma$.

Motion of the wetting front $X_3(t)$ in a three-dimensional spherically symmetric domain (when the wetted volume has a shape of the hemisphere) exhibits universal scaling behaviour with time t , such that $X_3(t) \propto t^{1/4}$, ultimately going to standstill at finite saturation levels $s_0 \approx 0.6\%$. This behaviour led us to a conjecture, confirmed in numerical simulations of the superfast diffusion model, that in general, depending on the geometry, basically on its dimension n , $X_n(t) \propto t^{1/(n+1)}$, which may be used in practical applications to analyse such kind of spreading processes.

the surface of grains was solely defined by the surface roughness, at least for the well-wetting liquid-solid combinations used in our study. Such universal behaviour allows to predict one of the main parameters of the models, s_0 with sufficient accuracy only on the basis of the effective surface area

$S_T / (1-R)$, porosity and the average amplitude of the surface roughness R .

One can then finally conclude that on the basis of comparison with experimental data the augmented superfast non-linear diffusion model (30) provides adequate description of liquid transport at low saturation levels, which therefore can be used in practical applications.

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APPENDIX: NUMERICAL MOVING MESH METHOD.

The numerical technique used to solve the partial differential equations in this study is a moving mesh method driven by conservation, similar to that presented in [37] and described in [38]. A nodal velocity v is constructed from a combination of a non-linear diffusion equation, for example the 3-D radially symmetric nonlinear diffusion equation

$$\frac{\partial s}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} r^2 D(s) \frac{\partial s}{\partial r};$$

and the conservation law

$$\frac{\partial s}{\partial t} + \frac{1}{r^2} \frac{\partial}{\partial r} r^2 s v = 0; \quad (39)$$

yielding the velocity formula

$$v(r; t) = - \frac{D(s)}{s} \frac{\partial s}{\partial r} \quad (40)$$

where $v(0; t) = 0$. An equation for ds/dt following the motion is then

$$\begin{aligned} \frac{ds}{dt} &= \frac{\partial s}{\partial t} + v(r; t) \frac{\partial s}{\partial r} = - \frac{1}{r^2} \frac{\partial}{\partial r} r^2 s v + v(r; t) \frac{\partial s}{\partial r} \\ &= - s \frac{1}{r^2} \frac{\partial}{\partial r} r^2 v = s \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{D(s)}{s} \frac{\partial s}{\partial r} \end{aligned} \quad (41)$$

Introducing moving nodes $b_i(t)$ and corresponding saturation values $s_i(t)$; ($i = 1; \dots; N$), an approximation to (40) is

$$v_{i+1/2}^n = - \frac{D(b_{i+1/2}^n)}{s_{i+1/2}^n} \frac{s_{i+1}^n - s_i^n}{b_{i+1}^n - b_i^n} \quad (42)$$

The system (41) is approximated by the first-order-in-time semi-implicit scheme

$$\begin{aligned} \frac{s_i^{n+1} - s_i^n}{\Delta t} &= \frac{s_i^n}{(b_{i+1/2}^n)^2 \frac{D(b_{i+1/2}^n)}{s_{i+1/2}^n} \frac{s_{i+1}^n - s_i^n}{b_{i+1}^n - b_i^n} \\ &\quad + \frac{s_i^n}{(b_{i-1/2}^n)^2 \frac{D(b_{i-1/2}^n)}{s_{i-1/2}^n} \frac{s_i^n - s_{i-1}^n}{b_i^n - b_{i-1}^n}} \end{aligned} \quad (43)$$

($i = 1; \dots; N-1$) where Δt is the time step, which has the property that no new local extrema in s_i are created in the interior of the domain in a time step, thereby preserving positivity of s_i and avoiding oscillations. This allows arbitrarily large numbers of nodes without Δt being restricted by stability conditions.

The scheme (43) can be written in the matrix form

$$B \underline{s}^{n+1} = \underline{s}^n \quad (44)$$

where $\underline{s}^{n+1} = [s_1^{n+1}, \dots, s_N^{n+1}]^T$, $\underline{s}^n = [s_1^n, \dots, s_N^n]^T$, and B is a tridiagonal matrix modified to take into account the boundary condition $s_N = s_f$ and the continuity condition $\partial s / \partial r = 0$ at $r = 0$.

Once the s_i^{n+1} have been obtained the mesh nodes b_i^{n+1} can be found from the Lagrangian form of the conservation principle (39), i.e.

$$\int_0^Z b(r; t) r^2 dr \text{ is constant in time,} \quad (45)$$

valid when $s(r; t) > 0$.

A discretisation of (45) is

$$f(b_{i+1}^{n+1})^3 s_{i+1}^{n+1} - (b_i^{n+1})^3 s_i^{n+1} = \text{its initial value} \quad (46)$$

($i = 2; \dots; N$), yielding b_i^{n+1} by recursion over i , given $b_0^{n+1} = 0$. Since the s_i^{n+1} are