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Department of Mathematics

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A ss rtaton su tt n parta u ntot r qur ntort r o astro n at at so nt an In ustra Co putaton August 2014

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Abstract

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1 Introduction

The migration of contaminants or reactants through porous redia is of critical importance for a wide variety of scienti c and industrial processes. This process can include both reaction with and without the porous media.¹ Contamination of soils and sands for example, by liquid pollutants can result in those pollutants entering groundwater systems, thus increasing the chance of harm to crops and exatems, and water supplies to the public. It is important therefore to characterise such phenomena, and be able to predict the fate of such species, dependent on poromedia and pollutant type, over a wide range of conditions. It is known that the nonlineadi usion of unreactive pollutants can be classi ed into slow, fast or superfast di usion, dependent on the characteristics of the di usion coe cient in the porous medium equation. The di usion coe cient is often dependent on the saturation level of the contaminant species in the porous medium, which drives the di usion. This changesver time as the solution 1.1 Background to di usion through porous media

is the porous medium equation (PME) in D Cartesian coordinates. It can be generally stated as

$$\frac{@u}{@t} = \frac{@}{@x} D (u(x(t);t)) \frac{@u}{@x} + s(x);$$

where D(u(x(t);t)) is the di usion coe cient (which, when $D(u) = u^m$, is the PME). For radial di usion, the nonlinear PME is given by

$$\frac{@u}{@t} = \frac{1}{r^{d-1}} \frac{@}{@r} u^m r^{d-1} \frac{@u}{@r} + s(r);$$
(1)

where d is the number of dimensions. In this study we take = 2. For both radial and cartesian coordinatess(x(t)) and s(r(t)) represent asource or sink term, such as ingress of another source of liquid into the system, or evapation of the liquid out of the system respectively. In the case of this study, we do not not respect or sink terms, particularly since we assume that our migrating quid is a non reacting, non volatile liquid.

The transition of transport through porous media is very mult dependent on the saturation level of the solvent. This change in di usion behavior can be very sharp as detailed in the study by Lukyanov et al [2]. This transition is seen to occur at about 20% saturation for low saturation levels. The general classification of the "speed" of non linear di usion with respect to the value of m (142 11.9551 Tf 2249375 atiliad)-0.902

for slow (m = 1) and superfast (m = 3=2) di usion. Where the concentration u(r) is greater than 20% of u(r = 0), for m = 1, we present a self similar/analytic solution for u(r(t);t), which is used to obtain the boundary values of the velocityd(r=dt), rate (@u=@and gradient (@u=@r







This paper provided evidence, from an environmental polliut perspective, that small concentrations of harmful solvents can travel long distates through packed soils/sands over long periods of time, thus justifying the requirement investigate the migration of harmful contaminant species.

The transport of liquid through the porous media was deduceted be due to capillary action at the surface-roughness scale of the individual ptionles, and indeed the total saturation of the sand is the interplay between that within the capillary bridges, and that in the surface roughness around the particles. Genately, the ow obeys a Darcy-like Law, where permeability is related to the geontery of the grooves [4]. In macroscopic modelling of the migration of the nonvolated liquid, it was assumed that the particles were perfect spheres, and that the wetter grooves within the surface roughness of the particles were completely lied. Modellignresults were then compared following non-dimensionalisation, for saturation, distace and time. When comparing to equation (1), = m + 1. This is known assuperfast di usion. In the standard porous medium equation (which we will use for the slow section of our model), where m > 1 in equation (3), the low saturation levels at the edge of theiduid delay the onset of the wetting front, however (and in our model for supreast di usion), for superfast regimes, the velocity of the wetting front decreaseover time as the saturation level/concentration decreases. The results of the modelæin agreement with experiment, and for the characterised system with the organic superfast diffusion regime is said to hold fo0:5% < s < 10%. It was also shown that the wetted volume, V fell on a power law with time, whereV / $t^{0:75}$ as shown in Figure 4.

occur where the solution value for concentration (or satution) is 20% of its maximum value. As expected, the central node will not move, however the other nodes in the mesh will move with a velocity that changes with time. This is a rst attempt at

In Chapter 4 we present the results of the moving mesh methods for both whand superfast di usion in isolation for 2D radial di usion, followed by the results for the combined numerical method. In the case of the slow di usion evolves the results for constant mass between spatial nodes. We discuss the stational limitations on the discretisation of time via a Lagrangian type Courant-Friedchs-Lewy (CFL) condition [7]. This condition prevents the spatial nodes from overtaining one another.

In Chapter 5 we draw some conclusions from the results, comparing the **basic** the slow and superfast regimes in isolation with the combinded usion moving mesh scheme.

In Chapter 6 we make recommendations for future study0.13dr315523T19(o)0.13069726(f63(c

2 Generation of an analytic solution for slow di usion

In this chapter we look for an analytic solution to the porousmedium equation where m = 1, by generating a self similar solution. We shall rstly desribe the scale invariance applied to2D radial di usion, and follow this with the generation of the self similar/analytic solution. This method is discussed in reference [8], and adopted in 1D Cartesian coordinates, where m = 4, in reference [9].

2.1 Scale invariance for slow di usion

We consider the case whene = 1 and d = 2 in the nonlinear porous medium equation (2)

$$\frac{@u}{@t} = \frac{1}{r^{d-1}} \frac{@}{@r} r^{d-1} u^m \frac{@u}{@r}$$
(2)

where d is the number of dimensions. We now apply a scaling transfo**rtion** to equation (2),

$$u = 0; t = f; r = r;$$
 (3)

using the scaling parameter, , where and are constants. This transforms equation (2) into the new non-dimensionalised variables, \hat{t} , and \hat{r} ;

$$-\frac{@?}{@?} = \frac{2 \quad 2}{n^{d-1}} \frac{@}{-1}$$

and

$$u(b) = 0$$
 at the boundary $r = b(t)$:

This results in

$$\frac{\overset{@}{@}^{Z} b(t)}{\overset{b(t)}{@} t_{0}} r^{d-1} u \, dr = 0;$$

$$\overset{Z}{\overset{b(t)}{}} r^{d-1} u \, dr = k; \qquad (6)$$

and so

where k is a constant. Upon transformation of equation (6) into a, t and t we obtain

$$\overset{d}{=} \begin{array}{c} Z_{b(t)} \\ \uparrow^{d-1} \hat{\mathbf{0}} d \hat{\mathbf{n}} = {}^{0} \mathbf{k}; \\ \end{array}$$

thus generating a second equation in and ,

$$+2 = 0:$$
 (7)

Therefore, solving equations (5) and (7)

$$=\frac{1}{4};$$
 and $=\frac{1}{2}:$

This results in a scale transformation

$$u = \frac{1}{2}0; t = t, and r = \frac{1}{4}t$$

SO

$$= \frac{u^{1=}}{0^{1=}} = \frac{t}{t} = \frac{r^{1=}}{t^{1=}}:$$

An in depth text on scaling methods and self similarity can be ound in reference [11].

2.2 Generation of a self similar solution for slow, nonlinear di usion

We now introduce two variables, and y, that are independent of , and which are invariant under transformation equation (3). We then make a function of y, and then transform as follows

$$= \frac{u}{t} = \frac{a}{t};$$

$$y = \frac{r}{t} = \frac{r}{t}$$

With

where d is a constant of integration. Therefore

$$= A \quad \frac{y^2}{8};$$

where A is a constant. We we can write

= A
$$\frac{y^2}{8}$$
; $\frac{y^2}{8}$ A:
= A $\frac{y^2}{8}$;

Figure 5 illustrates the self similar solution, equation ()3 where A = 2, for the original non-linear 2D equation (2), where d = 2, m = 1. Four time steps are shown. It can be seen that the pro le gradually attens over time and is symmetric about r = 0. In this study we take the initial time,

$$= ru \frac{@u^{r_{B}(t))}}{@r_{r_{A}(t)}} + ur \frac{dr}{dt}$$

Algorithm for slow di usion alone with mass conservation

Initially:

1. De ne the initial condition everywhere to be

$$u(r) = 2 - \frac{r^2}{8}$$
 at $t_0 = 1$

- Discretise the meshr_i(t) = r₀(t) + i r, where r are N uniform discretisations
 i = 0; 1; :::; N, across the domain att₀.
- 3. Calculate the initial masses between nodes using SimptsoRule $b_i = \frac{R_{r_i}}{r_0}$ urdr, between the origin atr₀, and nodesi, for i = 0;:::;N.

Then, at each time step,

1. Calculate the velocities from equation (12), approximating the gradient by suitable nite di erences, for example, central di erences:

$$\frac{@}{@}r_{i} = \frac{u_{i+1}(t) - u_{i-1}(t)}{r_{i+1}(t) - r_{i-1}(t)} \quad i = 1; \dots; N = 1;$$

2. De ne the velocity of the nal node at r_N through linear extrapolation

$$v_{\rm N} = 2 v_{\rm N} _{1} v_{\rm N} _{2}$$

or by using the one-sided di erence

$$v_N \qquad \frac{u_N \quad u_{N-1}}{r_N \quad r_{N-1}}:$$

3. Update the new positions at the next time step using the exipit Euler scheme

$$r_i(t + t) = r_i(t) + t \frac{dr}{dr_i};$$

for equally spaced time steps t.

4. Update the solutions at the next time step using the new pidisons from step 3,

$$u_{i}(t + t) = \frac{b_{i+1} - b_{i-1}}{r_{i}(t + t)(r_{i+1}(t + t) - r_{i-1}(t + t))}; \text{ for } i = 1; \dots; N - 1:$$

5. Calculate u at the origin by approximating the integral/mass between the origin and the rst mesh point at t + t,

$$Z_{r_1(t+t)} = ur dr = \frac{1}{4} (u_0(t+t) + u_1(t+t)) r_1(t+t)^2 r_0(t+t)^2 = b_1:$$

The value of b_1 is constant for all time. Therefore

$$u_0(t + t) = \frac{4b_1}{r_1(t + t)^2} u_1(t + t)$$

 $asr_0(t) = 0$ 8t.

6. Finally, the value of $u_N(t + t) = \frac{1}{5}u_0(t + t)$, from the boundary condition at $r_N 8t$.

Results are presented in Section 4.1.

At r_1 , it is assumed that the boundary values are given by the selfmilar solution u(r;t) = u(0;t)=5. The initial conditions are also taken to be the solutions to the self similar solution at $r_i(t)$. We start with the initial conditions

$$u_1 = \frac{2}{5}$$
 at $t_0 = 1$

therefore from equation (8)

$$r_0 = \frac{8}{p_{\overline{5}}}$$
 at $t_0 = 1$:

Also, from the self similar solution, substituting $t_0 = 1$ into the appropriate equations

$$\frac{@}{@}u_{1} = \frac{(r_{1})^{2}}{8}$$
 1 at t_{0} ;

and

$$\frac{@u}{@r_1} = \frac{r_1}{4} \text{ at } t_0:$$

We can also nd an expression for the initial velocity of the l_{0} w/fast interface, $r_{1}(t)$, from

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}\mathbf{t}} = \frac{\mathbf{@}\mathbf{u}}{\mathbf{@}\mathbf{r}} \cdot \frac{\mathrm{d}\mathbf{r}}{\mathrm{d}\mathbf{t}} + \frac{\mathbf{@}\mathbf{u}}{\mathbf{@}\mathbf{t}}$$

Since at the interface

$$\frac{du}{dt} = 0$$
 at time t;

then the velocity at the interface node is therefore given by

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}\mathbf{t}}_{\mathbf{I}} = \frac{\mathbf{@} \mathbf{u}}{\mathbf{@} \mathbf{t}_{\mathbf{I}}} \cdot \frac{\mathbf{@} \mathbf{u}}{\mathbf{@} \mathbf{r}_{\mathbf{I}}}$$
$$= \frac{\mathbf{r}_{\mathbf{I}}(\mathbf{t})}{2\mathbf{t}} \cdot \frac{\mathbf{4}}{\mathbf{r}_{\mathbf{I}}(\mathbf{t})} \mathbf{p}_{\overline{\mathbf{t}}} \quad \text{at } \mathbf{t}:$$
(13)

Due to the ux into the region at $r_1(t)$ (from what is the slow di usion regime)

$$ru \frac{@u}{@r} + ru \frac{dr}{dt} = 0$$
 at $r_1(t)$:

There is an additional boundary condition $atr_N(t)$, that maintains/drives migration

of the liquid.

$$u_b = 0:01$$
 at r_b ; t 0:

The total mass in the fast domain ($_{l}\left(t\right) ;r_{b}(t)$

integrals of u from $r_0(t)$ to $r_i(t)$, where $i = I (= 0); 1; \ldots; N$

at time t, we obtain

$$\frac{dr}{dt}_{i} = \frac{u_{i}r_{i}}{u_{i}r_{i}} (1 \quad i) \frac{dr}{dt}_{i} + \frac{(u_{i})^{m}r_{i}}{u_{i}r_{i}} (1 \quad i) \frac{@u}{@r_{i}} (u_{i})^{m-1} \frac{@u}{@r_{i}} (19)$$

Hence, calculating the velocity of the internal nodes at an**t** ime requires knowledge of the boundary values atr₁, i.e, u₁, $\frac{dr}{dt}$ and $\frac{@u}{@r_1}$, making use of the self similar solution. Using the previous equation (13), to recap

$$\frac{dr}{dt}_{1} = \frac{r_{1}}{2t} - \frac{4}{r_{1} - t} \text{ at time t}$$

and from our knowledge at the interface,

$$\frac{@}{@}u_{r_{1}} = \frac{r_{1}}{4t} \text{ and } \frac{@}{@}u_{1} = \frac{(r_{1})^{2}}{8t^{2}} \frac{1}{t^{3=2}};$$

we can substitute these into expressions into equation (19a) obtain

$$\frac{dr}{dt}_{i} = \frac{u_{i}r_{i}}{u_{i}r_{i}} (1 \quad i) \quad \frac{r_{i}}{2t} \quad \frac{4}{r_{i}\frac{p}{t}} + \frac{(u_{i})^{m}r_{i}}{u_{i}r_{i}} (1 \quad i) \quad \frac{r_{i}}{4t} \quad (u_{i})^{m-1} \quad \frac{@u}{@r}_{i} :$$

This is how the velocity of the spatial nodesr(t) progress in the superfast di usion domain.

We now seek a suitable time-stepping method for the superfaceoving mesh method, and update the position of each spatial node by

$$r_i(t + t) = r_i(t) + t \frac{dr}{dt};$$

and the total mass $_{fast}(t + t)$ by

$$fast(t + t) = fast(t) + t_{fast}^{0}(t);$$

where ${}^{0}_{fast}(t)$ is given by equation (15). We have expressions for bot ${}^{0}_{r_{1}}$ and ${}^{dr}_{dt_{1}}$ (derived from the self similar solution). So equation (15) ecomes

$$\int_{\text{fast}}^{0} (t) = \frac{(r_{1})^{2} u_{1}}{2t} \frac{(u_{1})^{m-1}}{2} + \frac{4u_{1}}{p} \frac{1}{\bar{t}} : \qquad (20)$$

We can now recover the solution for (r(t + t); t + t) at the next time step, approx-

imating equation (16) as

$$u_{i}(t + t) = _{fast}(t + t) \frac{i+1}{r_{i}(t + t)(r_{i+1}(t + t) - r_{i-1}(t + t))}$$
 (21)

The individual mass fractions ($_i$) do not change with time. The self similar solution is used to calculate values of (r; t) and the velocities of the spatial nodes y_i at time t = 0, at what would be the boundary with the slow di usion regime.

In the superfast region we can no longer use the self-similar value of the nal node between the nal node of the self similar solution/slow paraola, and the nal node in the superfast di usion pro le, where we have assigned a intervalue of u(N;t) = 0.01. We give the solution at the nal node this small value of u in order to ensure the advancement of the uid. In reality, where u(N;t) = 0 the capillary bridges in Figure 3 would collapse and no longer exist, and therefore the would be no further

The initial values of $u_i(t_0)$ in the fast di usion regime are given by

$$u_i = u_N + (u_1 - u_N) \frac{N - r + r_1 - r_i}{(N - r)^2}$$
: (22)

The total mass in the fast region, att_0 is therefo

3. De ne the boundary conditions $atr_1(t)$ at time t

$$u_1 = \frac{2}{p_{\overline{t}}} = \frac{r_1}{8t};$$
 as given by the self similar solution
 $v_1 = \frac{r_1}{2t} = \frac{4}{r_1 + \overline{t}};$ as given by the self similar solution

4. De ne the boundary conditions $atr_b(t)$

$$\mathbf{u}_{\mathrm{b}}$$

4. Compute the new total mass from $_{I}(t + t)$ to $r_{N}(t + t)$ using $_{fast}^{0}(t)$ calculated from Equation (20), and explicit Euler method.

$$fast (t + t) = fast (t) + \begin{pmatrix} 0 \\ fast \end{pmatrix} t$$

The boundary conditions at $r_0 = 0$, $t_0 = 1$ are

$$u_0 = 2;$$

$$\frac{@}{@}u_0 = 0;$$

$$\frac{dr}{dt}_0 = 0;$$

and for all time t > 0,

$$\frac{@u}{@r_0} = 0;; \qquad (23)$$

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t}_{0} = 0;; \qquad (24)$$

as, intuitively, the origin about which di usion is symmetric, $r_0(t)=0$.

Let us denote the position and solution at the interface between slow and superfast di usion as r_1 and u_1 respectively, at t_0 , where I is the spatial nodal identity. We know from previous equations (25), (26), (27), and (28) re**sp**tively, that at $t_0 = 1$ for an initial discretisation $r = \frac{1}{4^{1/2}} \frac{1}{5}$,

$$r_1 = \frac{8}{5}; \tag{25}$$

$$\frac{@u}{@r_1} = \frac{p_{\overline{5}}}{p_{\overline{5}}};$$
(26)

$$\frac{dr}{dt}_{+} = \frac{3^{6} \overline{5}}{10};$$
 (27)

$$\frac{@u}{@t_1} = \frac{3}{5}$$
 (28)

Howl.8)

Therefore, since

$$\frac{dr}{dt}_{0} = 0 \quad \text{and} \quad \frac{@u}{@r}_{0} = 0 \quad \text{at} \quad r_{0}(t) = 0$$
$$\frac{dr}{dt}_{i} = \frac{u_{i}r_{1}}{u_{i}r_{i}} \quad @u$$



Figure 6: Identi cation of velocity of interface node between slow and fast di usion regimes

There will be zero rate of change of mass as mass ows at the seamate into the superfast regime as ows out of the slow regime, by the app**aition** of the continuity equation at the boundary;

$$\frac{d}{dt} = \frac{1}{|slow(1)|} \sum_{r_{1}=1}^{Z} \frac{r_{1}(t)}{r_{1}=1(t)} ur dr + \frac{1}{|fast(1)|} \sum_{r_{1}=1}^{Z} \frac{r_{1}(t)}{r_{1}(t)} ur dr = 0:$$
(31)

where $_{slow(1)}$ and $_{fast (1)}$ represent the total mass in the slow and fast regimes respectively at time t_0 . The integral to the left of the boundary is given by

$$\frac{d}{dt} \frac{1}{|slow(1)|} \sum_{r_{1}=1}^{Z_{r_{1}}} ur dr = \frac{1}{|slow(1)|} \sum_{r_{1}=1}^{Z_{r_{1}}} \frac{@u}{@t} dr + ur \frac{dr}{dt} \Big|_{1=1}^{1} \frac{1}{(|slow(1)|)^{2}} \frac{d}{dt} \frac{|slow(1)|}{|t|} \sum_{r_{1}=1}^{Z_{r_{1}}} ur dr; \quad (32)$$

an tot r t t s

w r

$$A = \frac{u_{1}r_{1}}{slow(1)} \quad 1 \qquad \frac{(r_{1}^{2} - r_{1}^{2})(u_{1} + u_{1})}{4 slow(1)}$$
$$+ \frac{u_{1}^{m}r_{1}}{fast(1)} \quad \frac{(r_{1+1}^{2} - r_{1}^{2})(u_{1+1} + u_{1})}{4 fast(1)} \qquad I+1$$

an

$$B = \frac{u_{l} r_{l}}{slow(1)} \quad 1 \qquad \frac{(r_{l}^{2} \quad r_{l-1}^{2})(u_{l} + u_{l-1})}{4 \quad slow(1)}$$

+
$$\frac{u_{l} r_{l}}{fast (1)} \quad \frac{(r_{l+1}^{2} \quad r_{l}^{2})(u_{l+1} + u_{l})}{4 \quad fast (1)} \qquad l+1$$

). Co bining the initial pro le for slow and fast di usive regi es at initial ti e $t_0. \label{eq:theta}$

ow t	at w	av	pr	ss ons	or t	v	0	t	0	t	spat a	n no	s n t	S OW	us on	
r	quat	on 🔥	•	t sup	r ast	r			q	ıat	1	Ģ				

on



Figure 7: Combined slow and fast di usion profiles at t₀.

i. Generating an algorith for the co bined di usion.

now n rat ana ort to a van t nta pro sr n ton 📐

Combining slow and superfast di usion

For a s \mathbf{r}_i i = 0;:::;N

$$0 = r_0(t) < r_1(t) < \dots < r_1 < \dots < r_N(t) < r_N(t)$$

w sum or at t_0 wt N no sa stan r apart $r_N(t)$ n a ovn oun ar r nt ra no $r_1(t)$ st no at w t sow us on r an stot suprastr

In t a

 ${\rm At}\,t_0\ {\rm an} \quad {\rm v}\,{\rm n}\,t \quad {\rm oun}\ {\rm ar} \quad {\rm on}\ t\,{\rm on}$

 $u_{N}(t) = 0:01;$

Ca u at t v o t

From the output of the tensor of the tensor tensor

$$u_{N}(t + t) = 0:01:$$

Ca u at t so ut on at t or n $\boldsymbol{r_0}$

$$u_0(t + t) = \frac{4_{slow}(t + t)_1}{(r_2(t + t)^2)} u_1(t + t);$$

as sr n ton

Ca u at t up at sout on at t nt r a

$$u_{l}(t + t) = u t$$

4 Results







Fur r votsot nos ras wt nrasnt ant vot spat pro attnsout ssn pnwtt pr nta osrvatons tatast prorssst qu urt strot or $nr_0(t)$ w vntua stop w nt r sno on ran rvn prssur roqu nt ap ar r s s an a on pro ot as sr nr rn





on t rs o t nt ra

$$\frac{@\,u}{@\,r_1} \quad \frac{u_l \quad u_{l-1}}{r_1 \quad r_{l-1}} \quad \mathrm{on} \; slow \quad \mathrm{us} \; \mathrm{on} \; \mathrm{s} \quad \mathrm{o} \; \mathrm{nt} \; \mathrm{ra}$$

an

5 Discussion and Conclusions

In t s s t on w s uss t p at ons an on us ons ro t r su ts

The sprotasion attinura on no ot sowan suprast us on trou a porous un a two neona ra a o an to as one ron nonvoat nonratnesp san p tnt rn set to approat parta rvatves are protasion at suprast us on o a ovn set as on onstant assertons wire assert ntrest suprast o an rotinitian oun arise on ton wire as set soutonesus not sow of anto trinitiva value attintra

ovn s nt rn to as prov su ssun o nt pro o on ntraton ot sp sa anst spa ant owvrwt tatons on t t st p p n nt ont CF on ton

to or o n sow us on wt onstant assovrt o an as prov su ssu prov n t at t < 0:011 or t sp $r = \frac{1}{45}$ at t_0 s avo s spata no s ovrta n on anot r t us nsurn strn nt trqur nt tan t s p as o sow us on wt ontant ass For sta t n t s r t s r qur tat t < 5 10 5 s tat on s to a r to t CF on ton

 $\label{eq:linear} {\rm In} \ {\rm t} \ {\rm s} \quad {\rm t} \ {\rm o} \ {\rm t} \quad {\rm vau} \ {\rm o} \ u_l \left(t\right) \ {\rm at} \ {\rm t} \quad {\rm t} \ {\rm an} \quad {\rm oun} \ {\rm ar} \ {\rm o} \ {\rm t} \quad {\rm o} \ {\rm an} \ {\rm was}$

6 Recommendations for future work

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