Similarity Solutions for Solute Transport in Fractal Porous Media using a Time- and Scale-Dependent Dispersivity

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ABSTRACT

A specific form of the Fokker-Planck equation with a time- and scale-dependent dispersivity is presented for modelling solute transport in saturated heterogeneous porous media. By taking a dispersivity in the form of separable power law dependence on both time and scale, we are able to show the existence of similarity solutions. Explicit closed-form solutions are then derived for an instantaneous point-source (Dirac delta function) input, and for constant concentration and constant flux boundary conditions on a semi-infinite domain. The solutions have realistic behaviour when compared to tracer breakthrough curves observed under both field and laboratory conditions. Direct comparison with the experimental laboratory data of [1] shows good agreement between the source solutions and the measured breakthrough curves.

KEYWORDS: Time and scale dependent dispersivity, similarity solutions, fractal, heterogeneity.

1. Introduction

Transport of solute in the subsurface is controlled by many mechanisms including physical, chemical and biological activities. The Fokker-Planck equations are widely used models for quantitative investigation of transport processes. Their application entails the determination of model parameters, usually estimated using laboratory or field data. An unresolved issue in quantitative analysis of solute transport using the Fokker-Planck equation is that currently used forms do not account for the variability of parameters found in the field.

Usually contaminant transport models assume a constant dispersion coefficient that is calibrated separately for each different downstream sample location, resulting in different dispersion coefficients for the same flow problem. In an attempt to overcome this, alternative forms for the dispersion coefficient have been developed with a view to uniquely calibrate it across all sampling locations. In [2] a unique dispersion coefficient that was a function of the mean travel distance proved successful in modelling tracer data exhibiting scale effects. Another approach is to model dispersivity as being time dependent. Analytical solutions for time-varying dispersion coefficients have been presented by [3] in two dimensions and [4] in three dimensions. The mobile-immobile region model could be approximated by a one-dimensional advection-dispersion equation with effective time-dependent velocity and dispersion coefficient, through matching the zeroth-, first- and second-order moments of both models ([5]). Time-dependent dispersion coefficients are also used for describing nonclassical or anomalous dispersive transport. For example [6] used a power-law function to model dispersion in a fractal soil as did [7] and [8] for diffusion on a Sierpinski carpet.

Scale or spatially dependent dispersion models along with analytical solutions for instantaneous source and Dirichlet boundary conditions in one dimension can be found for a dispersivity proportional to the actual distance travelled, x, in [9], [10], [11] and [1]. Both [9] and [11] include the effect of molecular diffusion in their solutions. In the absence of an advection term, [12] modelled dispersion on a fractal domain where the dispersion coefficient was a power-law function of distance with the power dependent on the fractal dimension. Indeed, the concept of representing transport in natural soils as a fractal process is well established as a possible explanation to the scale-effect phenomenon ([13]). Extensive field tracer studies have revealed features of the scale effect ([14], [15], [16]) and the equally important issue of the time effect ([17], [18], [19], [20], [21]) as caused by porous media heterogeneity.

That dispersion in heterogeneous media is not described by a constant dispersion coefficient is now well accepted. To gain further theoretical understanding [22] looked at an intermediate flow regime between miscible and immiscible flow. In this region either theory should describe the flow and occurs in the limit of negligible molecular diffusion for miscible flow, and no interfacial tension in immiscible flow [22]. Working from the two-phase immiscible flow equations in the zero interfacial tension limit, they derive a convection-diffusion equation with a non constant dispersion term and therefore show theoretically that for one-dimensional flow, the dispersion coefficient is dependent on both flow length and flow velocity.

In [23] they note that it is inconsistent to use a classical advection diffusion equation whereby the concentration gradient is the driving force for the flux, when the mechanisms responsible for dispersion depend on velocity variation effects. They suggest that the effects of velocity fluctuations on dispersive mixing can be modelled through a dispersion coefficient which is a function of both space and time. Other research has led to the development of a nonlocal form of the flux to account for scale effects ([24], [25], [26]). Nonlocal flux relationships incorporate a flow memory such that " information from regions surrounding the mixing zone can alter the mixing profile" ([23]), and therefore provides a possible explanation as to "why dispersion appears dependent on the scale of measurement if the properties are also changing on this scale"

[23]. Experimental ([23], [26]) results from columns of multi-layered glass beds provide strong evidence to support a non-local model of dispersion.

While the scale and time effects of dispersion have generally been handled separately, there are a few papers on diffusion in fractal media which consider a dispersion coefficient that is a combined function of distance, x, and time, t. In [18], [27] and [28] a dispersion coefficient of the form $x^m t^\lambda$ was used to derive instantaneous source solutions. In our paper we extend their approach to the modelling of one-dimensional advective-dispersive transport by combining the fractal spatial model of [13] with the temporal model from [21]. This form of the dispersion coefficient includes the time-dependent dispersivity of [4] ($m = 0$), [2] ($m = 0$, $\lambda = 1$) and the scale-dependent form of [9], [10], and [1] ($m = 1$, $\lambda = 0$). Hence, to some extent the combined dispersion coefficient can be seen as generalising these three forms.

Analytical solutions are derived for three types of boundary conditions, an instantaneous point source, a constant concentration and a constant flux in a semi-infinite domain. All the solutions derived demonstrate known realistic behaviour as compared to tracer breakthrough curves observed under both field and laboratory conditions. We also show that the source solutions give good agreement with the experimental breakthrough curves of [1].

For further experimental evidence and theoretical investigations of scale and time effects, see ([29], [30], [31], [32], [33]), though these two issues tend to be addressed separately.

2. Solute transport equation

For the one-dimensional transport of a conservative solute in a saturated flow field, the governing equation is given by [34]

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(D \frac{\partial c}{\partial x} \right) - V \frac{\partial c}{\partial x}, \tag{1}$$

where c is the solute concentration, D is the hydrodynamic dispersion coefficient and V is the (constant) mean flow velocity (uniform porosity assumed). In order to incorporate the time and space components, the dispersion coefficient is written as (neglecting molecular diffusion)

$$D = \alpha(x,t)V^n = D_{\mathrm{o}} D_{\mathrm{x}}(x) D_{\mathrm{t}}(t)\, V^n, \tag{2}$$

where D_{o} is a constant, $D_{\mathrm{x}}(x)$ and $D_{\mathrm{t}}(t)$ are the spatial and temporal components of the dispersion coefficient respectively, n is a constant in the range $1 \le n \le 2$ ([34]) and α is the dispersivity.

In particular we take the following functional forms for $D_{\mathrm{x}}(x)$ and $D_{\mathrm{t}}(t)$

$$D_{\mathrm{x}}(x) = x^m, \tag{3}$$

$$D_{\mathrm{t}}(t) = t^{\lambda}, \tag{4}$$

which can be viewed as a combination of a fractal scale-dependent dispersivity developed by [13] and a temporal component of the dispersivity due to [21]. While [13] used $m = 2d - 1$ and gave $d = 1.0865$ though this was later modified by [33] to the range $1 < d < 2$. For $m = 1$, the dispersivity becomes a linear function of the scale. This is supported by a survey on published values of dispersivities conducted by [14]. For the time-dependent component [21] (p. 88) have suggested $-1 < \lambda < 0$.

Substitution of Eqs. (2), (3) and (4) into Eq. (1) results in

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(D_1 t^{\lambda} x^{m} \frac{\partial c}{\partial x} \right) - V \frac{\partial c}{\partial x}, \tag{5}$$

where $D_1 = D_o V^n$. We note that Eq. (5) also applies for non-conservative flow in the case of a linear absorption isotherm by replacing D_1 and V by D_1/R and V/R where R is the constant retardation factor. Alternatively, one can simply define t/R as a new time scale in Eq. (5). As discussed previously, Eq (5) with $V = 0$ has been used by [18], [27] and [28] to describe anomalous, non-classical diffusion or fractal diffusion on fractal domains.

3. Similarity solutions

In this section, we seek analytical solutions to Eq. (5). In particular we look for similarity solutions of the form

$$c(x,t) = \frac{f(\xi)}{t^a}, \qquad \xi = \frac{x}{t^b}, \tag{6}$$

where a and b are constants, subject to the initial and far-field boundary conditions

$$t = 0, \quad c = 0, \quad x > 0 \tag{7a}$$

$$x \to \infty, \quad \frac{\partial c}{\partial x} \to 0. \tag{7b}$$

We shall derive solutions for either a constant-concentration boundary condition at $x = 0$, i.e.,

$$x = 0, \quad c = c_o, \tag{7c}$$

a constant flux condition at $x = 0$,

$$x = 0\ , \quad Vc_{o} = Vc - D(0,t)\frac{\partial c}{\partial x}\,, \tag{7d}$$

or for an instantaneous source solution. Defining M to be the total mass of solute in solution at any given time

$$M = \int_0^{\infty} c(x,t)\, dx\ , \tag{8}$$

then, in addition we only consider instantaneous source solutions that are mass conserving.

Substituting Eq. (6) into Eq. (5) gives

$$-(af + b\xi f') = \frac{d}{d\xi}\left(t^{1+\lambda+b(m-2)} D_1 \xi^m f' - t^{1-b} V f\right), \tag{9}$$

where f' signifies $df/d\xi$. To obtain similarity solutions, Eq. (9) requires that

$$b = 1, \tag{10}$$

and

$$1 - \lambda - m = 0, \tag{11}$$

which enables Eq. (9) to be written as

$$-\left(af + \xi f'\right) = \frac{d}{d\xi}\left(D_1 \xi^m f' - Vf\right). \tag{12}$$

As mentioned earlier, [28] considered the same dispersion coefficient and similarity solutions as represented by Eq. (12) for modelling fractal diffusion in the absence of advection. In that case, similarity solutions require only that $b = (\lambda + 1)/(2 - m)$. Equations (10) and (11) give a dispersivity which behaves as $\alpha = D_o\, x^m\, t^{1-m}$, thus for $m = 1$ we have the case of $\alpha = D_o\, x$ ([11]

and [1]), while for $m = 0$ we have the case of $\alpha = D_o\, t$ ([2]). We note in Eq. (12) that a is an unspecified parameter. Its role is to differentiate between the instantaneous source solutions and the solutions arising from the other two boundary conditions given by Eqs (7c,d). These different types of solutions are now considered separately. It is also worthwhile noting that the units of D_1 depend on the parameter m and are given by $(\mathrm{L/T})^{2-m}$.

3.1 Instantaneous Source Solutions, $c(x,t) = f(\xi)/t$, $\xi = x/t$

From Eqs. (6), (8) and (10) we have

$$M = t^{1-a} \int_0^\infty f(\xi) d\xi \,, \tag{13}$$

which then requires $a = 1$ for the solutions to be mass conserving. Consequently, for these solutions M also represents the instantaneous source strength injected at $t = 0$. With $a = 1$, Eq. (12) is written as

$$-\frac{d}{d\xi}(\xi f) = \frac{d}{d\xi}\left(D_1 \xi^m f' - Vf\right), \tag{14}$$

which is solved subject to the condition derived from Eq. (7b)

$$\xi \to \infty, \quad f \to 0, \quad \frac{df}{d\xi} \to 0 \,. \tag{15}$$

Integrating Eq. (14), using Eq. (15) and rearranging results in

$$f' + (\xi^{1-m} - V\xi^{-m})\frac{f}{D_1} = 0 \,, \tag{16}$$

which can also be integrated directly to give

$$f(\xi) = \gamma \exp\left[\frac{V\xi^{1-m}}{(1-m)D_1} - \frac{\xi^{2-m}}{(2-m)D_1} \right], \quad m \neq 1, 2, \quad \lambda = 1-m, \tag{17a}$$

$$f(\xi) = \gamma \xi^{\frac{V}{D_1}} \exp\left(-\frac{\xi}{D_1} \right), \qquad m = 1, \; \lambda = 0, \tag{17b}$$

$$f(\xi) = \frac{\gamma}{\xi^{\frac{1}{D_1}}} \exp\left(-\frac{V}{D_1 \xi} \right), \qquad m = 2, \; \lambda = -1. \tag{17c}$$

In Eq. (17), γ is the constant of integration found by satisfying Eq. (13) (with a = 1). For various m, γ is given by

$$\gamma \; = \; M \Big/ \int_0^\infty \exp\left[\frac{V\xi^{1-m}}{(1-m)D_1} - \frac{\xi^{2-m}}{(2-m)D_1} \right] d\xi\,, \quad m \neq 1, 2, \; \lambda = 1-m, \tag{18a}$$

$$\gamma \; = \; \frac{M}{D_1^{1+V/D_1}\Gamma(1+V/D_1)}\,, \qquad m = 1, \; \lambda = 0, \tag{18b}$$

$$\gamma \; = \; \frac{M(V/D_1)^{\frac{1}{D_1}-1}}{\Gamma(1/D_1 - 1)}\,, \qquad m = 2, \; \lambda = -1. \tag{18c}$$

When m = 2, D_1 is dimensionless and γ is only defined for $D_1 < 1$. The case m = 1 is the solution presented by [10].

Finally the solutions for $c(x,t)$ are found by combining Eqs. (17) and (18) with (6) for a = b = 1 as

$$c(x,t)=\frac{M\exp\left(\dfrac{V\left(\frac{x}{t}\right)^{1-m}}{(1-m)D_1}-\dfrac{\left(\frac{x}{t}\right)^{2-m}}{(2-m)D_1}\right)}{t\int_0^\infty \exp\left[\dfrac{V\xi^{1-m}}{(1-m)D_1}-\dfrac{\xi^{2-m}}{(2-m)D_1}\right]d\xi}, \qquad m\neq 1,2,\ \lambda=1-m, \tag{19a}$$

$$c(x,t)=\frac{M}{t\,D_1^{1+V/D_1}\Gamma\left(1+V/D_1\right)}\left(\frac{x}{t}\right)^{V/D_1}\exp\left(-\frac{x}{D_1 t}\right), \qquad m=1,\ \lambda=0, \tag{19b}$$

$$c(x,t)=\frac{M\left(\dfrac{V}{D_1}\right)^{\frac{1}{D_1}-1}}{t\,\Gamma\left(1/D_1-1\right)\left(\dfrac{x}{t}\right)^{\frac{1}{D_1}}}\exp\left(-\frac{Vt}{D_1 x}\right), \qquad m=2,\ \lambda=-1. \tag{19c}$$

It is interesting to note that for m = 3/2 (d = 5/4 for [33]), Eq. (19a) can be fully integrated for γ. This integrable case also has additional physical significance as when $d=5/4$, (i.e., $d\approx 1.3$), the fractal dispersivity has been shown by [13] (Eq. (16), p. 571 – 572) to give the best fit to the field data from extensive tracer studies carried out under different conditions ([16]).

With m = 3/2 and, therefore, λ = -1/2, the integral in Eq. (18a) can be evaluated using Eq. (3.478-4) of [35] as

$$\int_0^\infty \exp\left(-\frac{2\xi^{1/2}}{D_1}-\frac{2V\xi^{-1/2}}{D_1}\right)d\xi = 4VK_2\left(\frac{4}{D_1}\sqrt{V}\right), \tag{20}$$

where $K_2\left(\frac{4}{D_1}\sqrt{V}\right)$ is the modified Bessel function of the second kind of order 2. Hence γ is given by $\gamma = M/4VK_2\left(\frac{4}{D_1}\sqrt{V}\right)$, and the solution for $c(x,t)$ is

$$c(x,t) = \frac{M}{4tVK_2\left(\frac{4}{D_1}\sqrt{V}\right)} \exp\left\{-\frac{2}{D_1}\left[\left(\frac{x}{t}\right)^{1/2} + V\left(\frac{x}{t}\right)^{-1/2}\right]\right\}, \quad m = \frac{3}{2}, \quad \lambda = \frac{-1}{2}. \tag{21}$$

For completeness we also note that Eq (19a) can be integrated for $m = 0$ whereby $\lambda = 1$. This is the case where the dispersivity is taken as proportional to the mean travel distance, or proportional to t. For $m = 0$ then we have

$$c(x,t) = \frac{M}{t\,\mathrm{erfc}(-V/\sqrt{D_1})}\sqrt{\frac{2}{\pi D_1}} \exp\left[-\frac{1}{2D_1}(x/t - V)^2\right], \qquad m = 0, \ \lambda = 1. \tag{22}$$

The dispersivity at the centre of mass of the plume where $x = Vt$, is, for all m, given by $\alpha \propto t$, hence the real effect of m on the above solutions is to change the shape of the plume around its peak concentration. Thus, m gives scope to reproduce the characteristic long time tail of scale dependent breakthrough curves. Finally, we see from Eqs. (16) and (17) that solutions satisfying the boundary condition of Eq (15) exist only for $m \le 2$. When $m > 2$, we still find that $f' \to 0$ as $\xi \to \infty$, but $f \to \gamma$ rather than zero and therefore do not correspond to a finite source strength.

3.2 Constant concentration boundary condition, $c(x,t) = f(\xi)$, $\xi = x/t$

When $a = 0$ it is then possible to find similarity solutions which satisfy a constant concentration boundary condition at $x = 0$. In this case, Eq. (12) becomes

$$f'' + \left(\frac{m}{\xi} + \frac{\xi^{1-m}}{D_1} - \frac{V\xi^{-m}}{D_1}\right) f' = 0\,, \tag{23}$$

which is solved subject to

$$\xi = 0\,, \qquad f = c_{\mathrm{o}}\,, \tag{24a}$$

$$\xi \to \infty\,, \quad f \to 0\,, \quad \frac{df}{d\xi} \to 0\,. \tag{24b}$$

Integrating Eq. (23) and using Eq. (24b) gives

$$\frac{df}{d\xi} \;=\; -\gamma\xi^{-m}\exp\left[\frac{V\xi^{1-m}}{(1-m)D_1} - \frac{\xi^{2-m}}{(2-m)D_1}\right]\,, \quad m \;\neq\; 1,2 \tag{25a}$$

$$\frac{df}{d\xi} \;=\; -\gamma\xi^{\frac{V}{D_1}-1}\exp\left(\frac{-\xi}{D_1}\right)\,, \qquad m = 1, \tag{25b}$$

$$\frac{df}{d\xi} \;=\; -\gamma\xi^{\frac{-1}{D_1}-2}\exp\left(\frac{-V}{D_1\xi}\right)\,, \qquad m = 2\,. \tag{25c}$$

For the next integration of each of Eqs. (25) we take each case separately.

3.2.1 $m \neq 1,2$ $\quad \lambda = 1 - m$

After a second integration of Eq. (25a) and using (24b) we have

$$f(\xi) \;=\; \gamma\int_{\xi}^{\infty}\zeta^{-m}\exp\left[\frac{V\zeta^{1-m}}{(1-m)D_1} - \frac{\zeta^{2-m}}{(2-m)D_1}\right]d\zeta\,, \tag{26}$$

which, after applying the boundary condition Eq. (24a), yields $f(\xi)$ as

$$f(\xi) \;=\; \frac{c_{\mathrm{o}}\int_{\xi}^{\infty}\zeta^{-m}\exp\left[\frac{V\zeta^{1-m}}{(1-m)D_1} - \frac{\zeta^{2-m}}{(2-m)D_1}\right]d\zeta}{\int_{0}^{\infty}\xi^{-m}\exp\left[\frac{V\xi^{1-m}}{(1-m)D_1} - \frac{\xi^{2-m}}{(2-m)D_1}\right]d\xi}\,. \tag{27}$$

3.2.2 $m = 1$ $\lambda = 0$

Integration of Eq. (25b) leads to

$$f(\xi) \;=\; \gamma D_1^{\frac{V}{D_1}} \int_{\frac{\xi}{D_1}}^{\infty} z^{\frac{V}{D_1}-1} e^{-z}\, dz\,, \tag{28}$$

which, along with Eq. (24a), gives $\gamma = c_{\text{o}} /[D_1^{V/D_1}\ \Gamma(V/D_1)]$. Therefore,

$$\begin{aligned} f(\xi) \;&=\; \frac{c_o}{\Gamma(\beta/D_1)} \int_{\frac{\xi}{D_1}}^{\infty} z^{\frac{\beta}{D_1}-1} e^{-z}\, dz \\ &= c_o \frac{\Gamma(\beta/D_1, \xi/D_1)}{\Gamma(\beta/D_1)}\,, \end{aligned} \tag{29}$$

where $\Gamma(\beta/D_1,\xi/D_1)$ is the incomplete gamma function. Eq (29) has also been previously derived by [11] and is given by their Eq. (34).

3.2.3 $m = 2$ $\lambda = -1$

Integrating Eq. (25c) results in

$$f(\xi) \;=\; \gamma \left(\frac{D_1}{V}\right)^{1+\frac{1}{D_1}} \int_0^{\frac{V}{D_1 \xi}} z^{\frac{1}{D_1}} e^{-z}\, dz\,, \tag{30}$$

and, from the boundary condition, $\gamma = c_{\text{o}} / \left[\left(D_1 / V \right)^{1+1/D_1}\ \Gamma(1+1/D_1) \right]$, thus

$$f(\xi) \;=\; c_{\text{o}} \left[1 - \frac{\Gamma\left(1+1/D_1, V/D_1\xi\right)}{\Gamma\left(1+1/D_1\right)} \right]. \tag{31}$$

3.2.4 $m = 0$ $\lambda = 1$

When $m = 0$, Eq. (27) is again fully integrable and gives

$$f(\xi) = \frac{c_o \operatorname{erfc}\left(\dfrac{\xi - V}{\sqrt{2D_1}}\right)}{\operatorname{erfc}\left(\dfrac{-V}{\sqrt{2D_1}}\right)} \quad . \tag{32}$$

3.2.5 m = 3/2 λ = -1/2

For m = 3/2, the integral in the denominator of Eq. (27) can be evaluated using Eq. (3.478-4) in [35] to give

$$f(\xi) = \frac{c_o\sqrt{V}}{4K_1(4\sqrt{V}/D_1)}\int_{\xi}^{\infty}\zeta^{-3/2}\exp\left(\frac{-2V\zeta^{-1/2}}{D_1} - \frac{2\zeta^{1/2}}{D_1}\right)d\zeta\ , \tag{33}$$

where $K_1\left(\frac{4}{D_1}\sqrt{V}\right)$ is the modified Bessel function of the second kind of order 1.

3.2.6 Complete Solutions

In summary then the full solutions for $c(x,t)$ for the different cases of m when a = 0 are given by Eqs. (6), (27), (29), (31), (32) and (33) as

$$c(x,t) = \frac{c_o\displaystyle\int_{x/t}^{\infty}\zeta^{-m}\exp\left[\frac{V\zeta^{1-m}}{(1-m)D_1} - \frac{\zeta^{2-m}}{(2-m)D_1}\right]d\zeta}{\displaystyle\int_0^{\infty}\xi^{-m}\exp\left[\frac{V\xi^{1-m}}{(1-m)D_1} - \frac{\xi^{2-m}}{(2-m)D_1}\right]d\xi}, \qquad m \neq 1,2 \tag{34a}$$

$$c(x,t) = \frac{c_o \operatorname{erfc}\left(\dfrac{x/t - V}{\sqrt{2D_1}}\right)}{\operatorname{erfc}\left(\dfrac{-V}{\sqrt{2D_1}}\right)} \quad . \qquad m = 0 \tag{34b}$$

$$c(x,t)=c_{\mathrm{o}}\frac{\Gamma\left(\dfrac{V}{D_1},\dfrac{x}{D_1 t}\right)}{\Gamma\left(\dfrac{V}{D_1}\right)}, \qquad m=1, \tag{34c}$$

$$c(x,t)=\frac{c_{\mathrm{o}}\sqrt{V}}{4K_1\left(\dfrac{4\sqrt{V}}{D_1}\right)}\int_{x/t}^{\infty}\zeta^{-3/2}\exp\left(-\frac{2V\zeta^{-1/2}}{D_1}-\frac{2\zeta^{1/2}}{D_1}\right)d\zeta \qquad m=\frac{3}{2}, \tag{34d}$$

$$c(x,t)=c_{\mathrm{o}}\left[1-\frac{\Gamma\left(1+1/D_1,Vt/D_1x\right)}{\Gamma\left(1+1/D_1\right)}\right], \qquad m=2. \tag{34e}$$

3.3 Constant flux boundary condition, $c(x,t) = f(\xi)$, $\xi = x/t$

Solutions for the solute flux boundary condition are given by having Eq (25) satisfy, from Eqs (2), (3), (4), (6) and (7d),

$$Vc_o = Vf-\left(D_1\xi^m f'\right)_{\xi=0}. \tag{35}$$

It is clear from Eq (25) that for $m \geq 1$, $\xi^m f'(\xi) \to 0$ as $\xi \to 0$, in which case Eq. (35) becomes identical to the constant concentration boundary condition. Hence, new solutions exist only for $m < 1$ where from Eq (25) $\xi^m f'(\xi) \to -\gamma$ as $\xi \to 0$. Applying Eq. (35) to Eq. (25a) results in $c(x,t)$ given by

$$c(x,t) \;=\; \frac{c_{\mathrm{o}}\int_{x/t}^{\infty}\zeta^{-m}\exp\left[\dfrac{V\zeta^{1-m}}{(1-m)D_1}-\dfrac{\zeta^{2-m}}{(2-m)D_1}\right]d\zeta}{\int_0^{\infty}\xi^{-m}\exp\left[\dfrac{V\xi^{1-m}}{(1-m)D_1}-\dfrac{\xi^{2-m}}{(2-m)D_1}\right]d\xi+\dfrac{D_1}{V}}, \qquad m<1, \tag{36}$$

which, in the case of $m = 0$, becomes

$$c(x,t) = \frac{c_o \operatorname{erfc}\left(\frac{x/t - V}{\sqrt{2D_1}}\right)}{\operatorname{erfc}\left(\frac{-V}{\sqrt{2D_1}}\right) + \frac{1}{V}\sqrt{\frac{2D_1}{\pi}} \exp\left(\frac{-V^2}{2D_1}\right)} . \qquad m = 0 \qquad (37)$$

In Table 1 summarises all of the similarity solutions derived in the previous sections for the different boundary conditions and the combinations of the two fractal parameters.

4. Discussion

4.1 Comparison of Instantaneous Source Solutions with Experimental Data

To test the applicability of the source solutions given in the previous sections we use the experimental data of [1]. Only a brief outline of the experiments is given here, full details are to be found in their paper. A conservative tracer, tritium, was injected into a saturated column over a finite time period and scaled (c/c_o) breakthrough curves were measured at x = 2, 4, 6 and 8 m downstream. The data from these breakthrough curves are shown in Fig. 1. As noted in [1] and shown in their Fig. 7, the water flow rate through the column was compromised at the early stages of the experiment and it was not until 2 h into the experiment that the flow rate returned to a constant value. Since breakthrough at x = 2 m and x = 4 m commenced just after 1 h and 2 h, respectively, these data are not reliable for validating the solutions and therefore more emphasis is placed on the x = 6 and 8 m breakthrough data. The time period for the tritium injection at 9 min was much less than the travel time for the solute to reach either x = 6 or 8 m. Hence, as far as the breakthrough curves at x = 6 and 8 m are concerned, the tritium could have been injected as an instantaneous source and therefore we can use the solutions presented in section (3.1). From Eq. (6) with $a = b = 1$, the data in Fig. 1 can be used to construct $f(\xi)$ as shown in Fig. 2. It is clear that the x = 6 m and 8 m data obey similarity while the x = 4 m data does not quite make similarity for reasons given earlier.

Since the peak concentration occurs at $\xi = V$, then, from Fig. 2, V = 1.4 m h^{-1}. The scaled mass of solute, M/c_o, within the column can be calculated from the curves in Fig. 4 of [1] as M/c_o = 0.21 m. Fig. 2 shows the results of curve fitting the parameter D_1 for m = 0, 1 and 2 from Eqs. (17), (18) and (22). Interestingly, we see very little difference between the curves for different values of m. In fact, it suggests that the effect of m can be compensated through D_1. One could say that there is no way of distinguishing which of the three sets of m and D_1 parameters is the best. They are all equally plausible for this data set. It is probably not surprising that around the peaks the curves all look exactly the same since the position of the concentration peak is occurring at $x = Vt$, hence the dispersion coefficient at the peak behaves as $D_1 x^m t^{1-m} = D_1 V^m t$. Thus, if we reduce D_1 by $1/V$ ($\cong$ 0.71) and $1/V^2$ ($\cong$ 0.5) for m = 1 and 2 respectively, the dispersion coefficient is exactly the same at the peak concentration.

In Figs. 1 and 2 we see very little effect due to the parameter m since the advective term in Eq. (5) tends to dominate the dispersive term for the duration of the experiment. In Fig. 3 we reduce the flow velocity by an order of magnitude and plot the breakthrough curves at x = 4 and 8 m. As in the previous figures the values for D_1 are chosen to have the same peak concentration for the different m. With the lower flow velocity the effect of m on the shape of the curves, and particularly the elongation of the breakthrough tail, is more significant. The smaller the value of m, the later the breakthrough commences and the greater the long time tail.

4.2 Constant Concentration and Flux Boundary Conditions

In Figs. 4 and 5 we plot the profiles for the constant concentration boundary conditions for various m and V = 0.1 m h^{-1}. The values of D_1 are chosen to show the effect of differences in magnitude between V and D_1 on the shape of the profiles. Fig 4 shows that for a high ratio of V/D_1 = 50 m^{m-1} h^{1-m}, the profiles become steeper as m increases with the steepness of the profile being due to the dominance of advection over dispersion. For V/D_1 > 10,000 the profiles are essentially independent of m and given by an abrupt front positioned on $\xi = V$. For lower ratios as shown in Fig 5, not only does the shape of the profiles vary considerably with m, but also the mass of solute within the profile and the surface gradient. From Eq. (25) the following cases can be classified for the behaviour of the gradient f' as $\xi \to 0$

(i) $m = 0$, $f'(0) = -\gamma$

(ii) $0 < m < 1$, $f'(0) = -\infty$

(iii) $m = 1$, $0 < V/D_1 < 1$, $f'(0) = -\infty$

$V/D_1 = 1$, $f'(0) = -\gamma$

$V/D_1 > 1$, $f'(0) = 0$

(iv) $m > 1$, $f'(0) = 0$.

Consequently, a large range of behaviour in the shape of the concentration profiles can be obtained through the parameters m, V and D_1. It is interesting to note that there is not a smooth transition in the behaviour of $f'(0)$ for various m across all the cases above. This is due to the dispersion coefficient being zero at $x = 0$ for m nonzero in which case Eq. (5) is singular. When $m = 0$ this singular behaviour disappears due to D being no longer dependent on x but only a function of t. By including molecular diffusion within the dispersion coefficient for $m > 0$ the singular behaviour would of course be removed but at the expense of obtaining straightforward analytical similarity solutions. In the case of m = 1, [9] and [11] were able to include molecular diffusion and find analytical solutions by Laplace transform techniques. It is unlikely that this technique would work for $m \neq 1$ due to the explicit appearance of t^{1-m} in the dispersion coefficient.

To determine the solute mass within the profile, we integrate Eq. (5) over x from zero to ∞ along with the boundary conditions Eqs. (7b) and (7c), and rewrite in terms of the similarity variables giving

$$\frac{\partial}{\partial t}\int_0^\infty \frac{c(x,t)}{c_\mathrm{o}}\,dx = \int_0^\infty \frac{f(\xi)}{c_\mathrm{o}}\,d\xi = V - \left[\frac{D_1}{c_\mathrm{o}}\xi^m f'(\xi)\right]_{\xi=0} \quad . \qquad (38)$$

As discussed earlier $\xi^m f'(\xi) \to 0$ as $\xi \to 0$ for $m \geq 1$, whereby Eq. (38) reduces to $\int_0^\infty f(\xi)/c_\mathrm{o}\,d\xi = V$. When $m < 1$, $\xi^m f'(\xi) \to -\gamma$ as $\xi \to 0$ and the solute mass within the profile is therefore greater than Vt since Eq. (38) becomes $\int_0^\infty f(\xi)/c_\mathrm{o}\,d\xi = V + D_1\gamma/c_\mathrm{o}$. For $m = 0$ we have

$$\frac{V}{\sqrt{D_1}} + \frac{\gamma\sqrt{D_1}}{c_\mathrm{o}} = \frac{V}{\sqrt{D_1}} + \sqrt{\frac{2}{\pi}}\,\frac{\exp\left(\dfrac{-V^2}{2D_1}\right)}{\mathrm{erfc}\left(\dfrac{-V}{\sqrt{2D_1}}\right)} \quad , \qquad (39)$$

and, with $V/\sqrt{D_1} = 0.1$, Eq. (39) gives $V/\sqrt{D_1} + \gamma\sqrt{D_1}/c_\mathrm{o} = 0.853$ being much greater than 0.1. However as the ratio $V/\sqrt{D_1}$ increases, the right-hand side of Eq. (39) approaches $V/\sqrt{D_1}$.

Figure 6 shows the shape of the concentration profiles for the flux boundary condition when m = 0 (Eq. (37)) as a function of the dimensionless distance $\xi/\sqrt{2D_1}$ with a range of values for the dimensionless parameter $V/\sqrt{2D_1}$. If $V/\sqrt{2D_1} < 2$, the concentration at the x = 0 boundary will always be less than c_0, but when $V/\sqrt{2D_1} \geq 2$ the exponential term in the denominator of Eq. (37) becomes negligible and the profiles are then identical to those from a constant concentration boundary condition given by Eq. (34b).

5. Summary

In this paper we have used a Fokker-Planck equation with a spatially and temporally varying dispersion coefficient for modelling solute transport in steady, saturated subsurface flow through heterogeneous porous media. This new dispersion coefficient generalises the traditional constant dispersion coefficient widely used for modelling transport processes in many fields.

For a Dirac delta function input, a constant-concentration input and a constant flux at the boundary, similarity solutions are obtained with simple explicit closed forms found for the parameter combinations of (m = 0, λ = 1), (m = 1, λ = 0), (m = 3/2, λ = -1/2) and (m = 2, λ = -1). The case m = 3/2, λ = -1/2 conforms to an average spatial fractal dimension of $d = 5/4 \approx 1.3$ found in extensive field and laboratory experiments ([13]). It was found that for the source solutions, m has a significant effect on the shape of the solute plume at large distances from the source for high flow velocities, and for essentially all x for low flow velocities. In the case of a constant concentration maintained at x = 0, a much greater effect of m on the shape of the concentration profiles is observed through both the surface concentration gradient and the mass of solute contained within the profile. It was shown that for $m > 1$, $f'(0) = 0$ while for $0 \leq m \leq 1$,

$f'(0) = 0$, $-\gamma$ or $-\infty$. Finally, the mass of solute contained within the profile for $0 \le m < 1$ is always greater than the solute mass for $m \ge 1$.

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Notation List

a	=	parameter (Eq. (6))
b	=	parameter (Eq. (6))
c	=	solute concentration (kg m^{-3})
c_o	=	solute concentration at x = 0
d	=	fractal parameter from Wheatcraft and Tyler (1988)
D	=	hydrodynamic dispersion coefficient (Eq. (2))
D_o	=	constant (Eq. (2))
D_1	=	$D_o V^n$ = constant
D_x	=	spatial component of the dispersivity (Eq. (2))
D_t	=	temporal component of the dispersivity (Eq. (2))
f	=	similarity function (Eq. (6))
K_1	=	modified Bessel function of the second kind of order 1
K_2	=	modified Bessel function of the second kind of order 2
m	=	dispersivity parameter (Eq. (3))
M	=	total mass of solute in solution (Eq. (8))
n	=	parameter (Eq. (2))
R	=	retardation factor
x	=	distance (m)
t	=	time (h)
V	=	mean water flow velocity (m h^{-1})
α	=	dispersivity (Eq. (2))
γ	=	constant of integration
λ	=	dispersivity parameter (Eq. (4))
ξ	=	similarity variable (Eq. (6))
Γ	=	gamma function

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Table 1

Dispersion Coefficient	**Source Solution** ***a* = 1**	**Constant Concentration at *x* = 0** ***a* = 0**	**Constant Flux at *x* = 0** ***a* = 0**
$m \neq 1,\ 2,\ \lambda = 1\text{-}m$ $D_1 x^m t^{1\text{-}m}$	$c(x,t)=\dfrac{M\exp\left(\dfrac{V\left(\dfrac{x}{t}\right)^{1-m}}{(1-m)D_1}-\dfrac{\left(\dfrac{x}{t}\right)^{2-m}}{(2-m)D_1}\right)}{t\int_0^\infty \exp\left[\dfrac{V\xi^{1-m}}{(1-m)D_1}-\dfrac{\xi^{2-m}}{(2-m)D_1}\right]d\xi}$	$c(x,t)\ =\ \dfrac{c_o\int_{x/t}^\infty \zeta^{-m}\exp\left[\dfrac{V\zeta^{1-m}}{(1-m)D_1}-\dfrac{\zeta^{2-m}}{(2-m)D_1}\right]d\zeta}{\int_0^\infty \xi^{-m}\exp\left[\dfrac{V\xi^{1-m}}{(1-m)D_1}-\dfrac{\xi^{2-m}}{(2-m)D_1}\right]d\xi}\ ,$	$c(x,t)\ =\ \dfrac{c_o\int_{x/t}^\infty \zeta^{-m}\exp\left[\dfrac{V\zeta^{1-m}}{(1-m)D_1}-\dfrac{\zeta^{2-m}}{(2-m)D_1}\right]d\zeta}{\int_0^\infty \xi^{-m}\exp\left[\dfrac{V\xi^{1-m}}{(1-m)D_1}-\dfrac{\xi^{2-m}}{(2-m)D_1}\right]d\xi+\dfrac{D_1}{V}}\ ,$
$m = 0,\ \lambda = 1$ $D_1 t$	$c(x,t)=\dfrac{M}{t\,\mathrm{erfc}(-V/\sqrt{D_1})}\sqrt{\dfrac{2}{\pi D_1}}\exp\left[-\dfrac{1}{2D_1}(x/t-V)^2\right]$	$c(x,t)\ =\ \dfrac{c_o\mathrm{erfc}\left(\dfrac{x/t-V}{\sqrt{2D_1}}\right)}{\mathrm{erfc}\left(\dfrac{-V}{\sqrt{2D_1}}\right)}$	$c(x,t)\ =\ \dfrac{c_o\mathrm{erfc}\left(\dfrac{x/t-V}{\sqrt{2D_1}}\right)}{\mathrm{erfc}\left(\dfrac{-V}{\sqrt{2D_1}}\right)+\dfrac{1}{V}\sqrt{\dfrac{2D_1}{\pi}}\exp\left(\dfrac{-V^2}{2D_1}\right)}$
$m = 1,\ \lambda = 0$ $D_1 x$	$c(x,t)=\dfrac{M}{t\,D_1^{1+V/D_1}\Gamma(1+V/D_1)}\left(\dfrac{x}{t}\right)^{V/D_1}\exp\left(-\dfrac{x}{D_1 t}\right)$	$c(x,t)=c_o\dfrac{\Gamma\left(\dfrac{V}{D_1},\dfrac{x}{D_1 t}\right)}{\Gamma\left(\dfrac{V}{D_1}\right)}$	

m = 3/2, λ = -1/2 $D_1 x^{3/2} t^{-1/2}$	$c(x,t) = \frac{M}{4tVK_2\left(\frac{4}{D_1}\sqrt{V}\right)} \exp\left\{-\frac{2}{D_1}\left[\left(\frac{x}{t}\right)^{1/2} + V\left(\frac{x}{t}\right)^{-1/2}\right]\right\}$	$c(x,t) = \frac{c_o\sqrt{V}}{4K_1\left(\frac{4\sqrt{V}}{D_1}\right)} \int_{x/t}^{\infty} \zeta^{-3/2} \exp\left(-\frac{2V\zeta^{-1/2}}{D_1} - \frac{2\zeta^{1/2}}{D_1}\right) d\zeta$	
m = 2, λ = -1 $D_1 x^2 t^{-1}$	$c(x,t) = \frac{M\left(\frac{V}{D_1}\right)^{\frac{1}{D_1}-1}}{t\,\Gamma(1/D_1 - 1)\left(\frac{x}{t}\right)^{\frac{1}{D_1}}} \exp\left(-\frac{Vt}{D_1 x}\right)$	$c(x,t) = c_o\left[1 - \frac{\Gamma(1+1/D_1, Vt/D_1 x)}{\Gamma(1+1/D_1)}\right]$	

1